Supplementary Information (SI)
for

Environmental potential of carbon dioxide utilization in the polyurethane supply chain

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Contents

1. Process data for PUR supply chain

	foam production		Synthesis of polyols			CO and H_2 supply			Methanol synthesis				Methane supply		Isocyonate production	
	Flexible PUR foam	Rigid PUR foam	Polyoxymethlyen (POM) units	Polycarbonate (PC) units	Polyether (PE) units	Reverse water gas shift	Dry reforming of methane	Steam methane reforming	CO_2-based	Steam methane reforming (SMR)	SMR+CO_2 Import	Combined reforming	Sabatier reaction	Natural gas	Toluol-2.4-diisocyanate (TDI)	Methylene diphenyl diisocyanate (MDI)
Reference	[1]	[1]				[2]	[3]	[2]	[4]	[1]	[5]	[1]	[6]	[7]	[8]	[8]
Inputs and outputs (Matrix A)																
Flexible foam [kg]	1															
Rigid foam [kg]		1														
Polyol [kg]	-0,713	-0,386	1	1	1											
Starter [kg]			-0,026	-0,026	-0,026											
Formaldehyde [kg]			-0,974													-30,03
Methanol [kg]									1	1	1	1				
Propylene oxide [kg]				-0,554	-0,974											
CO_2 [kg]				-0,420		-1,581	-0,910		-1,375		-0,36		-2,939			
H_2 [kg]						-0,072	0,050	0,216	-0,1875				-0,506			-8,07
Methane [kg]							-0,260	-0,724		-0,62	0,37	-0,574	1	1		
Benzene [kg]																-156,22
Toluene [kg]															-92,14	
Electricity [MJ]	-1,5	-1,5				-5,848	-7,305	-3,852	-4,572	-0,468	-1,0	-0,464	-1,188		-2302,9	-1991,1
Heat [MJ]						-2,468	1,770	-8,144			-2,2	-1				
Oxygen [kg]												-0,514				
CO [kg]						1	1	1							-56,02	-56,02
Nitric acid [kg]															-126,02	-126,02
Pentane [kg]		-0,054														
TDI [kg]	-0,285														174,16	
MDI [kg]		-0,616														250,26
Environmental impacts (Matrix B)																
GW [kg CO_2 eq.]	0,051					0,010	0,053	0,414	0,046	0,33		0,203	0,194	0,480		
FD [kg oil eq.]														1,310		
Amount CO_2 utilized (Vector d^T)																
CO_2 [kg]				0,420		1,581	0,910		1,375		0,36		2,939			

Table S 1 Process data for PUR supply chain

	Formaldehyde supply															
	Formaldehyde (Silver total)	Formaldehyde (Silverpartial)	Formaldehyde (Oxide/ Formox)	Pentane	Propylene oxide	Starter	Benzene	Toluene	Nitric acid	Electricity	Oxygen	Heat	CO_2 supply	H_2 supply	Functional unit vector	
Reference	[9]	[9]	[9]	[8]	[8]	[7]	[8]	[8]	[7]	[7]	[1]	[7]			f_{flex}	f_{rigid}
Inputs and outputs (Matrix A)																
Flexible foam [kg]															1	0
Rigid foam [kg]															0	1
Polyol [kg]															0	0
Starter [kg]						1									0	0
Formaldehyde [kg]	1000	1000	1000												0	0
Methanol [kg]	-1205,5	-1205,5	-1152,5												0	0
Propylene oxide [kg]					1										0	0
CO_2 [kg]													1		0	0
H_2 [kg]														1	0	0
Methane [kg]															0	0
Benzene [kg]							1								0	0
Toluene [kg]								1							0	0
Electricity [MJ]	-360	-360	-765							1	-2,88				0	0
Heat [MJ]	7756	2631,5	5540									1			0	0
Oxygen [kg]											0,231				0	0
CO [kg]															0	0
Nitric acid [kg]									1						0	0
Pentane [kg]				1											0	0
TDI [kg]															0	0
MDI [kg]															0	0
Environmental impacts (Matrix B)																
GW [kg CO_2 eq.]	134	134	54	1,105	3,140	8,37	1,86	1,21	1,900	0,133		0,068	var.	var.		
FD [kg oil eq.]				2,020	2,030	3,47	1,84	1,52	0,343	0,039		0,029	var.	var.		
Amount CO_2 utilized (Vector d^T)																
CO_2 [kg]																

Table S 1 (continued) Process data for PUR supply chain

2. Additional figures for flexible PUR foam

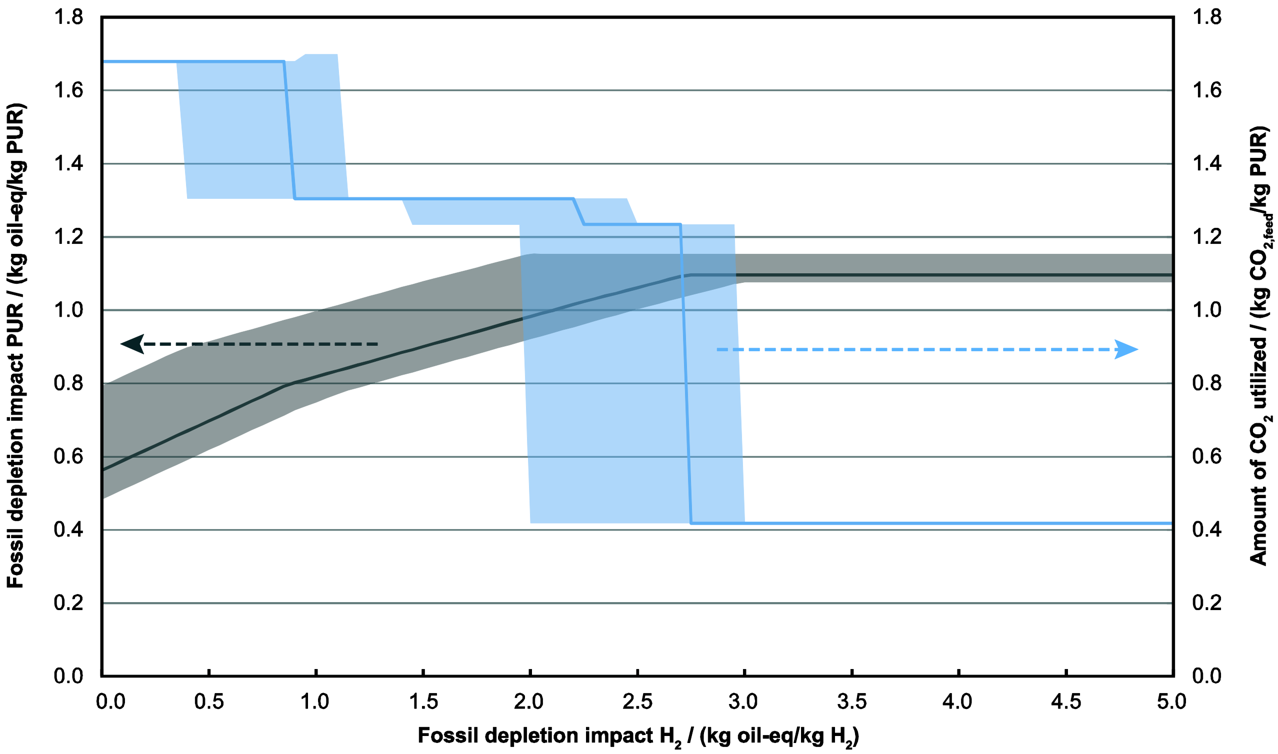

Figure S 1 Minimum fossil depletion impacts for flexible PUR foam for a variable fossil depletion impact of hydrogen production. The solid lines refer to CO_2 captured from a coal-fired power plant. The lower bound of the global warming impact of PUR and the upper bound of the CO_2 utilization amount refer to an ideal CO_2 source (best case). The upper bound of the global warming impact of PUR and the lower bound of the CO_2 utilization amount refer to CO_2 capture from ambient air (worst case).

3. Additional figures for rigid PUR foam

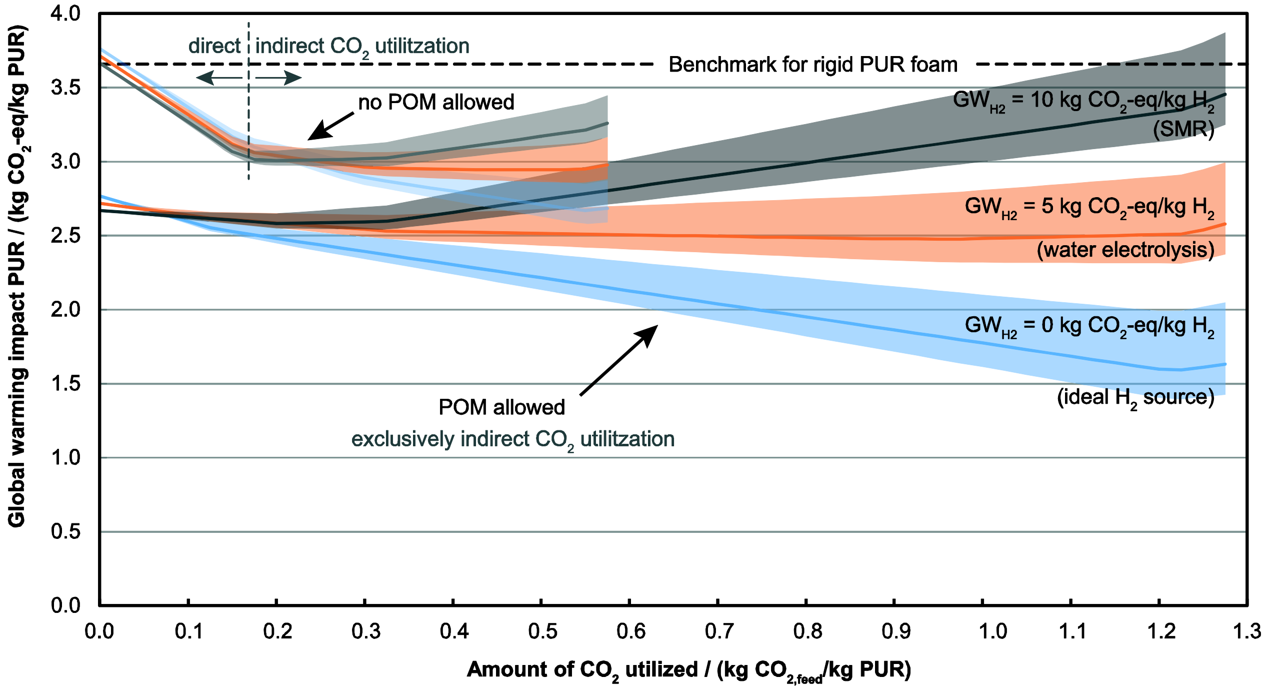

Figure S 2 Minimum global warming impact for rigid PUR foams for variable amounts of CO_2 utilized. The transparent areas indicate the range for alternative CO_2 sources: lower bounds correspond to an ideal source, upper bounds correspond to CO_2 capture from ambient air, and the solid lines correspond to CO_2 capture from a coal-fired power plant.

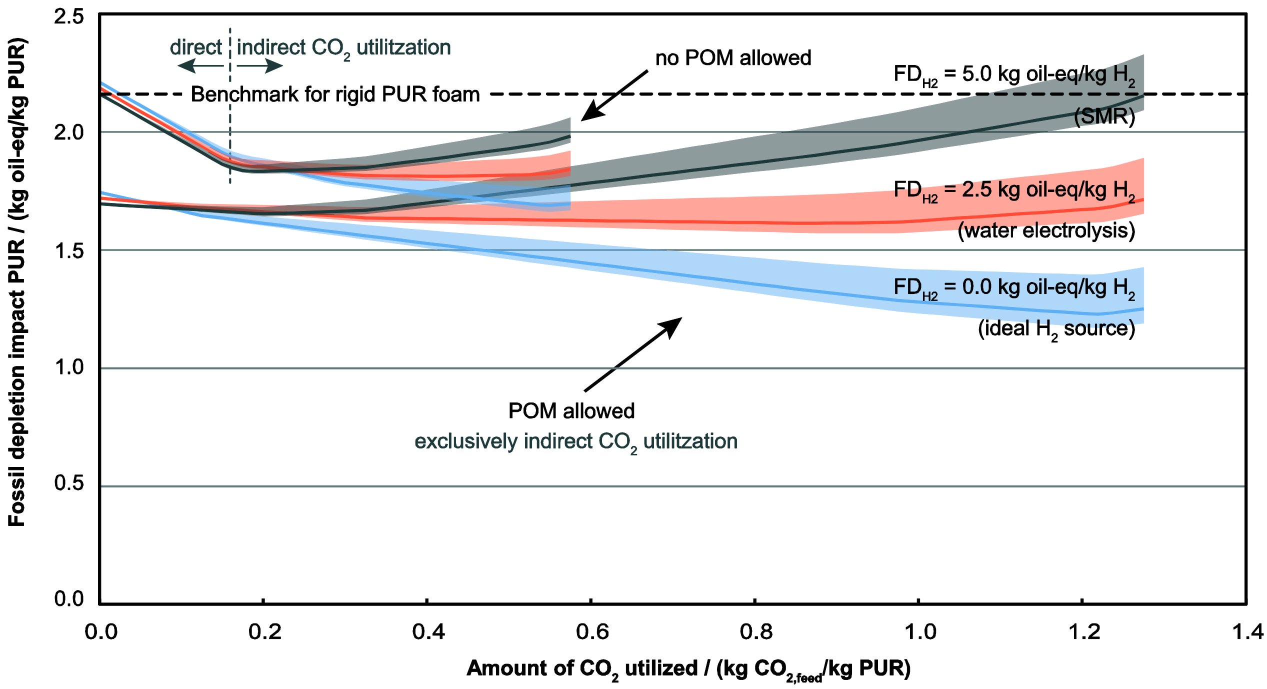

Figure S 3 Minimum fossil depletion for rigid PUR foams for variable amounts of CO_2 utilized. The transparent areas indicate the range for alternative CO_2 sources: lower bounds correspond to an ideal source, upper bounds correspond to CO_2 capture from ambient air, and the solid lines correspond to CO_2 capture from a coal-fired power plant.

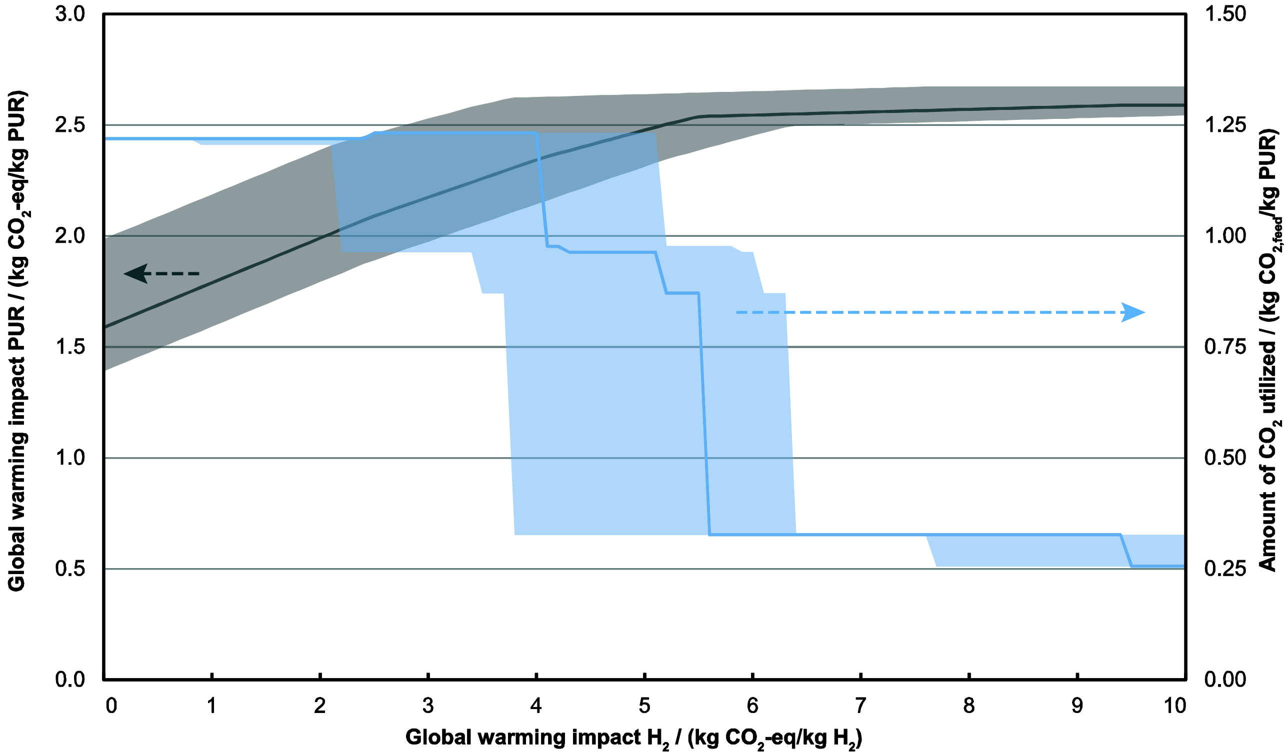

Figure S 4 Minimum global warming impacts for rigid PUR foam for a variable global warming impact of hydrogen production. The solid lines refer to CO_2 captured from a coal-fired power plant. The lower bound of the global warming impact of PUR and the upper bound of the CO_2 utilization amount refer to an ideal CO_2 source (best case). The upper bound of the global warming impact of PUR and the lower bound of the CO_2 utilization amount refer to CO_2 capture from ambient air (worst case).

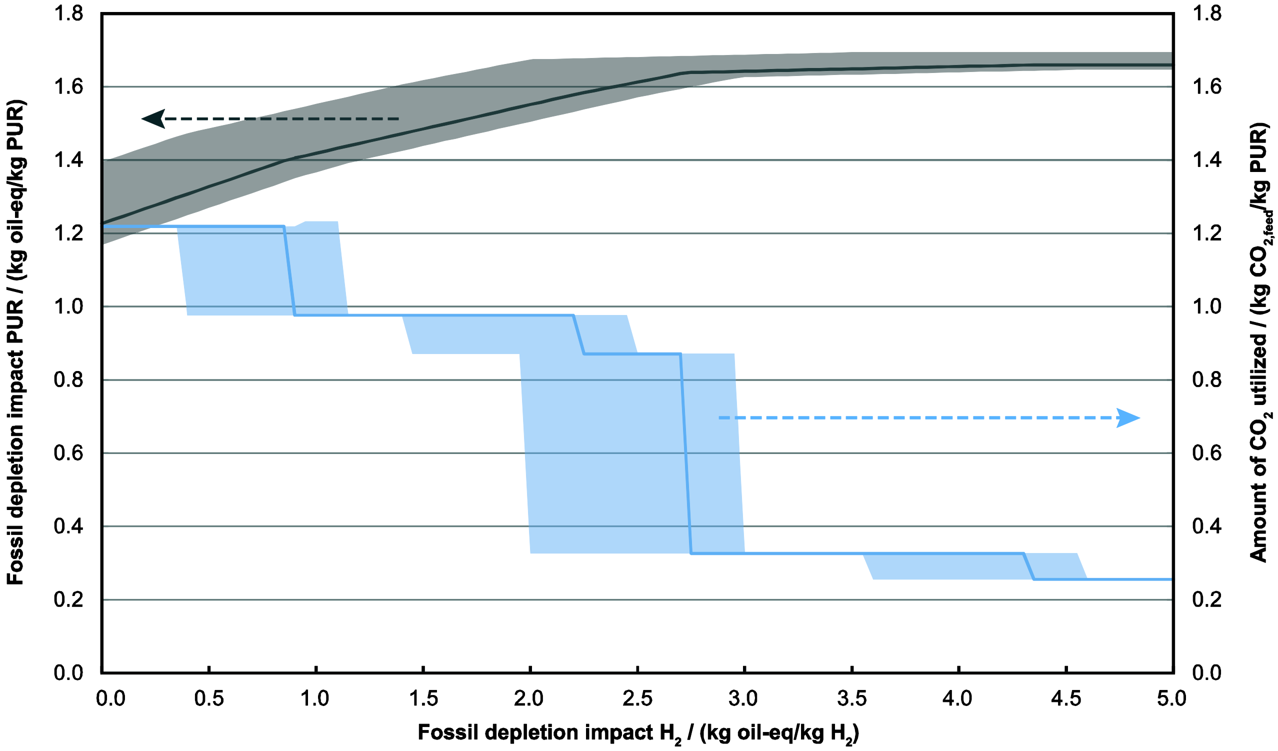

Figure S 5 Minimum fossil depletion impacts for rigid PUR foam for a variable fossil depletion impact of hydrogen production. The solid lines refer to CO_2 captured from a coal-fired power plant. The lower bound of the global warming impact of PUR and the upper bound of the CO_2 utilization amount refer to an ideal CO_2 source (best case). The upper bound of the global warming impact of PUR and the lower bound of the CO_2 utilization amount refer to CO_2 capture from ambient air (worst case).

References

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