Ex-ante Life Cycle Assessment of polyols using carbon captured from industrial process gas

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Supporting information

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Calculations

a) Estimation of emissions for the thermal oxidation processes

Emissions for thermal oxidation of the waste stream from polyols production for scenario 3 were estimated as follows: The waste stream is composed of dioxane, ethylene oxide (EO), and ethanal. Stoichiometric calculations were done to estimate emissions coming from the combustion (reaction with O_2) of these chemicals.

Thermal oxidation of dioxane ($C_4H_8O_2$)
m ($C_4H_8O_2$) = 2847.70 g

$C_4H_8O_2 + 5O_2 \rightarrow 4CO_2 + 4H_2O$

M ($C_4H_8O_2$) = 88.11 g/mol

n ($C_4H_8O_2$) = $\frac{2847.70\ g}{88.11\ \ g/mol}$ = 32.32 mol

m (CO_2) = 32.32 mol *4 * 44.01 g/mol = 5689.61 g = 5.69 kg

m (H_2O) = 32.32 mol * 4 * 18.02 g/mol = 2329.63 g = 2.33 kg

Thermal oxidation of EO (C_2H_4O)
m (C_2H_4O) = 85545.03 g

M (C_2H_4O) = 44.05 g/mol

$2C_2H_4O + 5O_2 \rightarrow 4CO_2 + 4H_2O$

n (C_2H_4O) = $\frac{85545.03\ g}{44.05\ g/mol}$ = 1942.00 mol

m (CO_2) = 1942.00 mol * 2 * 44.01 g/mol = 170934.84 g = 170.93 kg

m (H_2O) = 1942.00 mol * 2 * 18.02 g/mol = 69989.68 g = 69.99 kg

Thermal oxidation of ethanal (CH_3CHO)
$CH_3CHO + 2.5O_2 \rightarrow 2CO_2 + 2H_2O$

m (CH_3CHO) = 5695.41 g

M (CH_3CHO) = 44.05 g/mol

n (CH_3CHO) = $\frac{5695.41\ g}{44.05\ g/mol}$ = 129.29 mol

m (CO_2) = 129.29 mol * 2 * 44.01 g/mol = 11380.11 g = 11.38 kg

m (H_2O) = 129.29 mol * 2 * 18.02 g/mol = 4659.61 g = 4.66 kg

The same calculation procedure was used to calculate emissions for thermal oxidation of the waste stream from the intermediate production in scenario 3, and for the thermal oxidation of the waste streams in scenario 1 and scenario 2.

LCA data

The aggregated LCA data for gas conditioning[1,2] and the CCU polyols[3] production in scenarios 1, 2 and 3 are shown in the tables Table SI 1, Table SI 2, and Table SI 3. Chemicals were excluded from the tables due to the confidentiality issues.

Table SI 1 LCA inputs and outputs for scenario 1: selective catalytic combustion and CO-based polyol production (including intermediate production).

	Ecoinvent process	Value	Unit
Economic inputs			
Electricity	[G5013] electricity, medium voltage market group for electricity, medium voltage [RER]	$3.02*10^7$	kWh
Steam	[G14660] heat, from steam, in chemical industry market for heat, from steam, in chemical industry [RER]	$8.25*10^7$	MJ
Economic outputs			
CO-based polyol		$5*10^7$	kg
Environmental resources			
Cooling water	[E702] Water, cooling, unspecified natural origin [('natural resource', 'in water')]	$7.80*10^6$	m^3
Environmental emissions			
Water	Water [('water',)]	$7.80*10^6$	m^3
Carbon dioxide	Carbon dioxide, fossil [('air', 'non-urban air or from high stacks')]	$7.44*10^6$	kg

Table SI 2 LCA inputs and outputs for scenario 2: selective catalytic combustion, CO-based polyol production (including intermediate production) and CO_2-based polyol production.

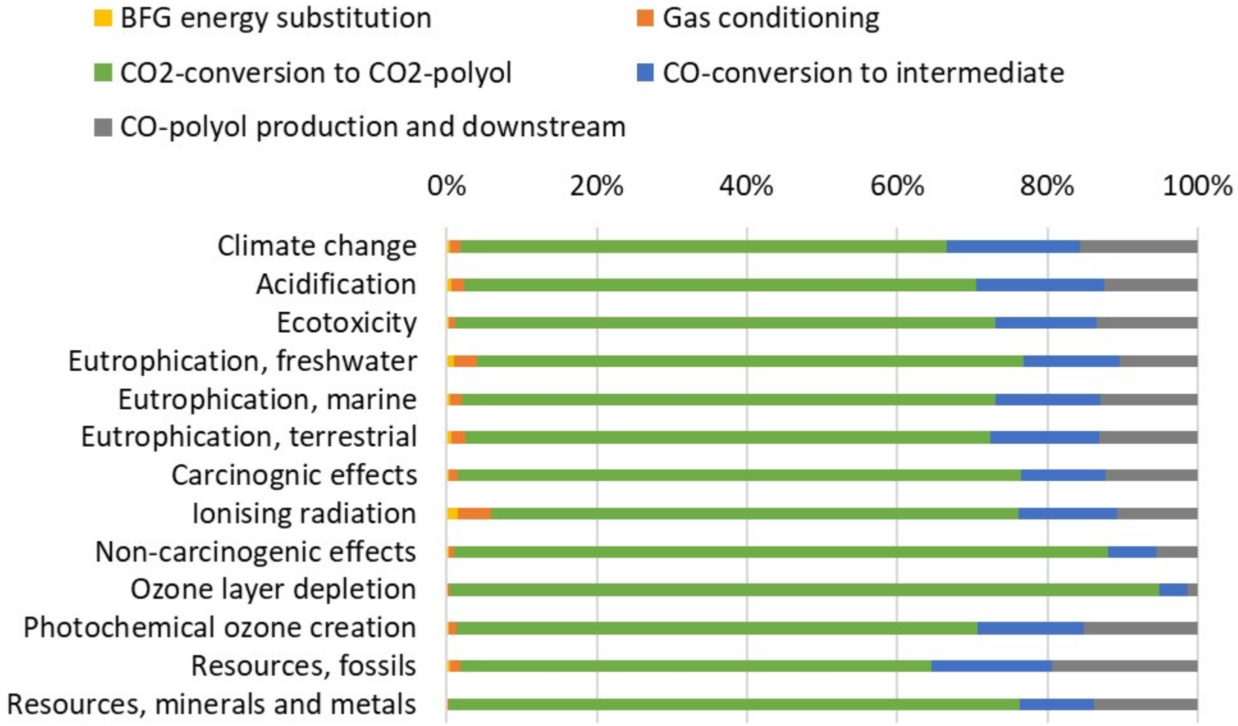
	Ecoinvent process	Value	Unit
Economic inputs			
Electricity	[G5013] electricity, medium voltage market group for electricity, medium voltage [RER]	$7.48*10^7$	kWh
Steam	[G14660] heat, from steam, in chemical industry market for heat, from steam, in chemical industry [RER]	$8.66*10^7$	MJ
Economic outputs			
CO-based polyol		$5*10^7$	kg
CO_2-based polyol		$9.93*10^7$	kg
Environmental			

resources			
Cooling water	[E702] Water, cooling, unspecified natural origin [('natural resource', 'in water')]	$1.20*10^7$	m^3
Environmental emissions			
Water	Water [('water',)]	$1.20*10^7$	m^3
Carbon dioxide	Carbon dioxide, fossil [('air', 'non-urban air or from high stacks')]	$7.61*10^6$	kg

Table SI 3 LCA inputs and outputs for scenario 3: chemical looping (with CO_2 removal), CO-based polyol production (including intermediate production) and CO_2-based polyol production.

	Ecoinvent process	Value	Unit
Economic inputs			
Electricity	[G5013] electricity, medium voltage market group for electricity, medium voltage [RER]	$6.49*10^7$	kWh
Steam	[G14660] heat, from steam, in chemical industry market for heat, from steam, in chemical industry [RER]	$6.45*10^7$	MJ
Heat	[G14480] heat, district or industrial, natural gas market group for heat, district or industrial, natural gas [RER]	$2.11*10^8$	MJ
Economic outputs			
CO-based polyol		$5*10^7$	kg
CO_2-based polyol		$1.11*10^8$	kg
Environmental resources			
Cooling water	[E702] Water, cooling, unspecified natural origin [('natural resource', 'in water')]	$1.17*10^7$	m^3
Environmental emissions			
Water	Water [('water',)]	$1.17*10^7$	m^3
Carbon dioxide	Carbon dioxide, fossil [('air', 'non-urban air or from high stacks')]	$1.32*10^7$	kg

Figures



a)

b)

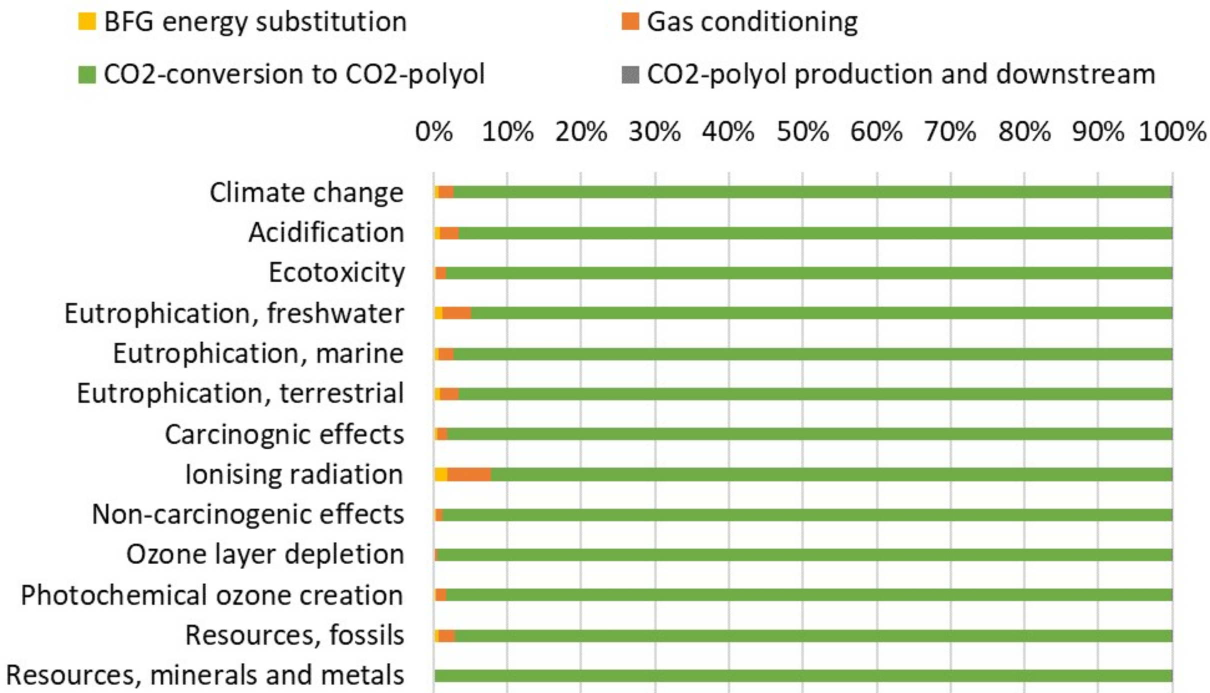
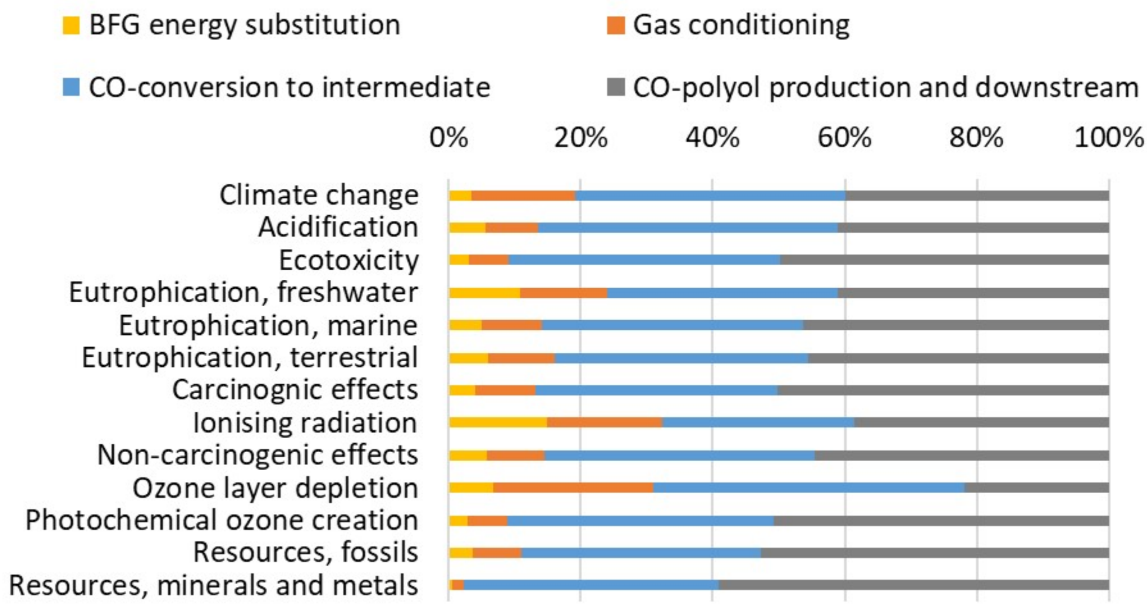


Figure SI 1 Contribution analysis results by processing steps for a) CO-based polyol and b) CO_2-based polyol for scenario 2.

a)



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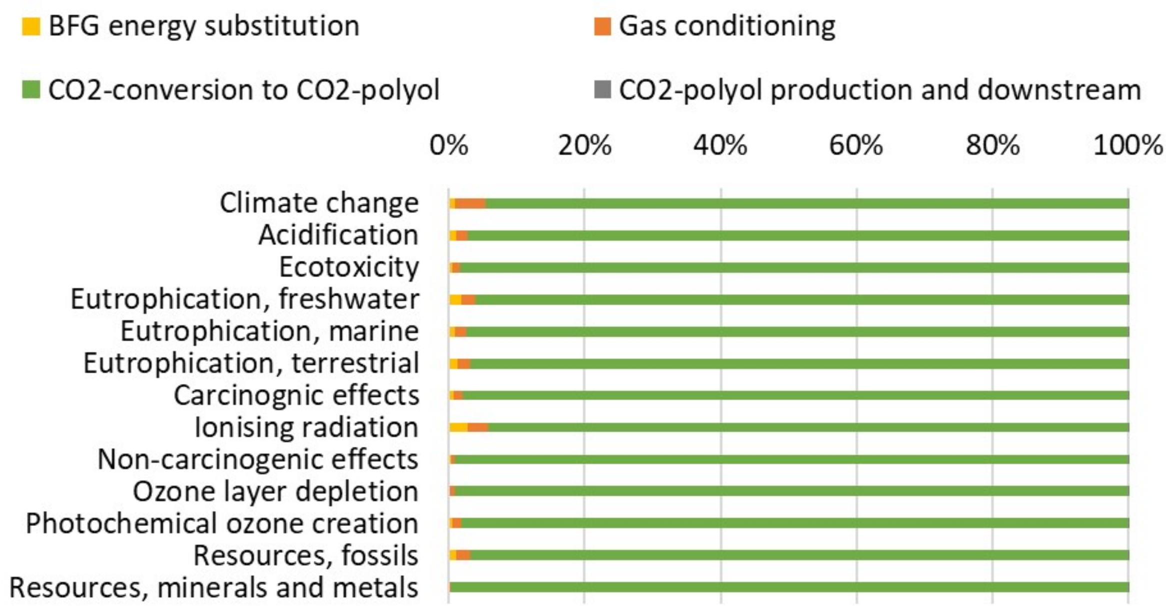
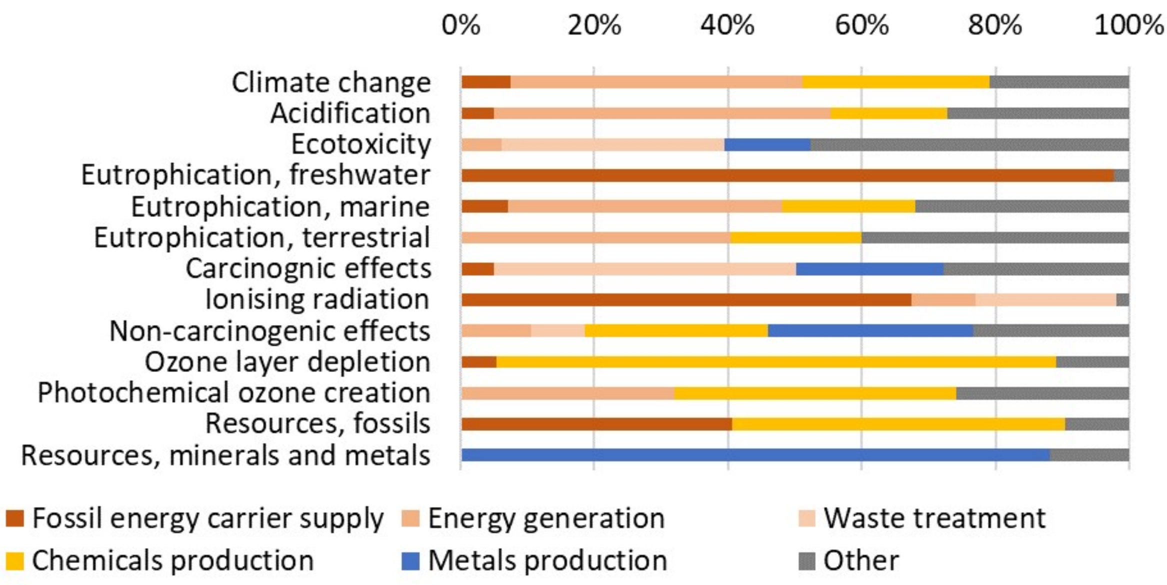


Figure SI 2 Contribution analysis results by processing steps for a) CO-based polyol and b) CO_2-based polyol for scenario 3.

a)



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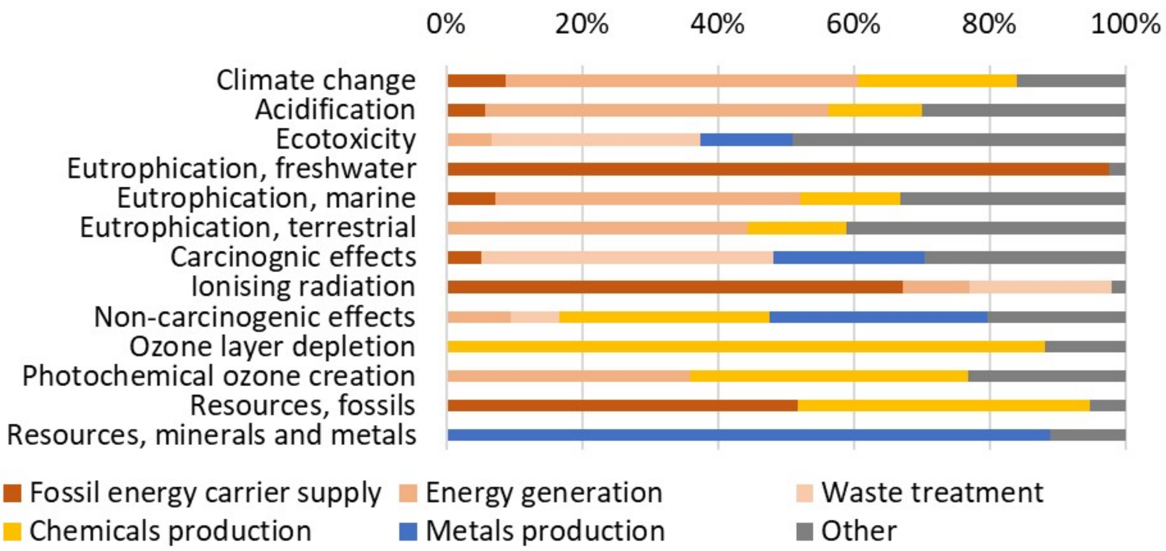
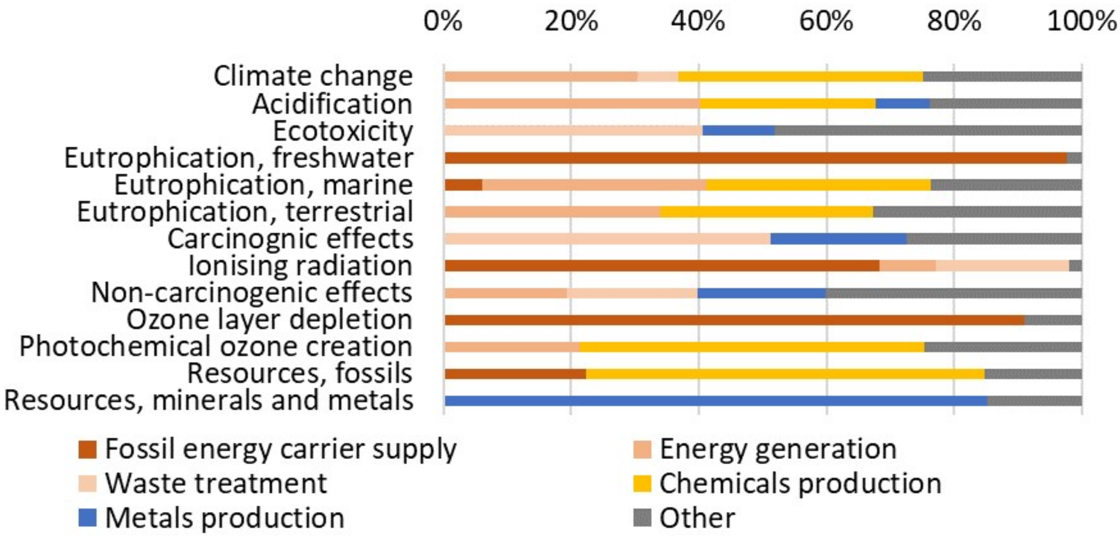


Figure SI 3 Contribution analysis results by sectors for a) CO-based polyol and b) CO_2-based polyol for scenario 2.

a)



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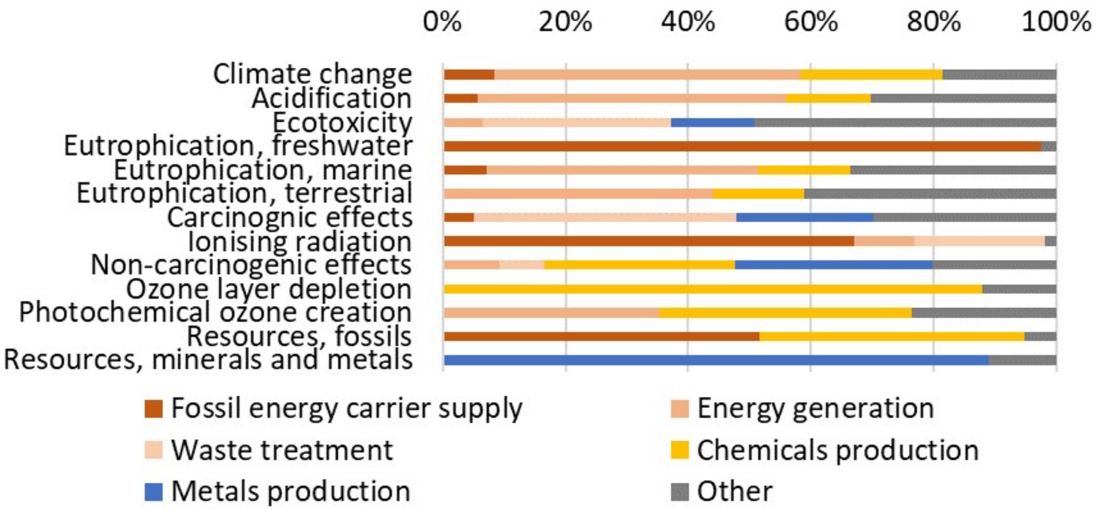

Figure SI 4 Contribution analysis results by sectors for a) CO-based polyol and b) CO_2-based polyol for scenario 3.

References

1 M. Aly, T. G. Gambu, Y. Zhang, V. V. Galvita and M. Saeys, *ACS Catal*, 2022, **12**, 9011–9022.

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