Procedural life cycle inventory of chemical products at laboratory and pilot scale: a compendium

Daniele Cespi,[a,b,*]

[a] *Department of Industrial Chemistry "Toso Montanari", University of Bologna, Viale Del Risorgimento 4, 40136, Bologna (BO), Italy*
[b] *Center for Chemical Catalysis - C3, Alma Mater Studiorum Università di Bologna, Viale del Risorgimento 4, Bologna (BO), Italy*

Corresponding author: Daniele Cespi, daniele.cespi2@unibo.it

Electronic supporting information (ESI)

Table S 1 – Average energy consumption values in MJ/kg for solvent recovery. Data were extrapolated from literature.[45]

Solvent type	n° C atom	n° H atom	MM (kg/kmol)	Boiling point (°C)	Vapor pressure (Torr)	Heating (MJ/kg)	Cooling (MJ/kg)	Tot. (MJ/kg)
Methanol	1	4	32.04	64.50	97.00	2.08	1.93	4.01
Ethanol	2	6	46.07	78.37	44.63	1.67	1.49	3.15
Acetic acid	2	4	50.05	118.00	15.70	0.66	0.55	1.21
Acetone	3	6	58.08	56.00	184.50	0.97	0.88	1.86
Isopropyl alcohol	3	8	60.10	82.00	32.40	1.39	1.19	2.58
THF	4	8	72.11	66.00	142.00	0.84	0.73	1.57
DMF	3	7	73.09	153.00	2.70	1.01	0.73	1.74
Ethyl ether	4	10	74.12	34.00	442.00	0.69	0.64	1.32
Hexane	6	14	86.18	69.00	124.00	0.72	0.59	1.31
Ethyl acetate	4	8	88.11	77.00	73.00	0.81	0.68	1.49
Toluene	7	8	92.14	110.60	28.50	0.67	0.49	1.16
Chloroform	2	1	119.38	61.20	158.40	0.49	0.43	0.92
1,2-dichlorobenzene	6	4	147.00	180.00	1.20	0.84	0.64	1.48

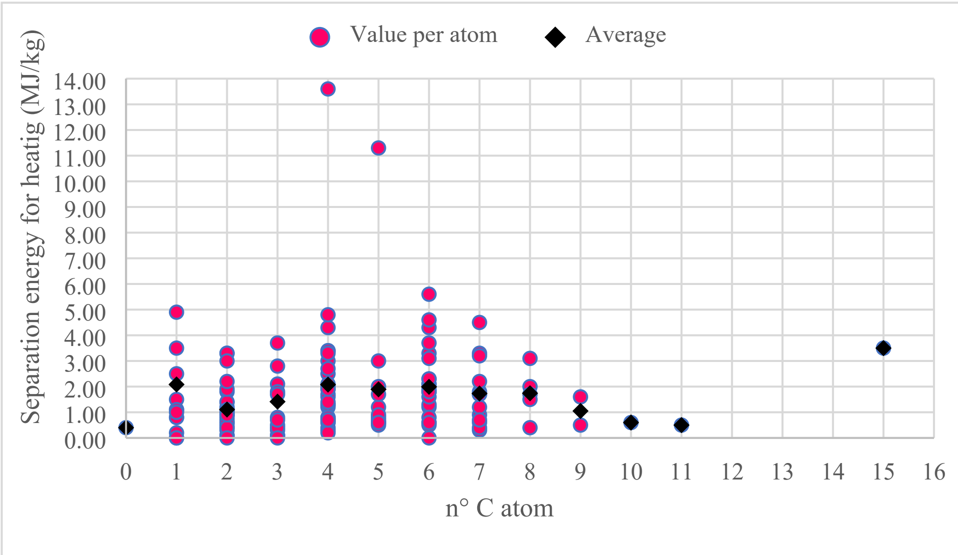
Table S 2 – Average energy consumption values in MJ/kg respect the number of H atoms. Data were extrapolated from literature.[20]

n° H atom	Average values in MJ/kg			
	separation energy		total energy	
	heating	cooling	heating	cooling
0	0.8	-1.8	1.6	-2.8
1	2.1	-2.9	2.4	-3.9
2	2.3	-4.4	4.6	-9.8
3	1.3	-2.5	2.7	-4.5
4	1.9	-3.7	3.4	-8.6
5	1.0	-1.5	1.6	-2.6
6	1.7	-2.7	3.6	-4.3
7	1.3	-2.5	2.6	-4.1
8	2.1	-2.8	3.6	-3.5
9	3.1	-4.7	4.7	-6.6
10	1.2	-1.6	2.2	-2.8
11	1.7	-4.2	4.0	-4.9
12	2.0	-2.3	2.7	-3.4
14	1.9	-2.4	2.9	-3.3
15	0.2	-2.1	1.7	-2.5
16	2.0	-1.3	2.5	-1.6
22	0.6	-0.8	1.1	-2.6

Table S 3 – Average energy consumption values in MJ/kg respect the number of C atoms. Data were extrapolated from literature.[20]

n° C atom	Average values in MJ/kg			
	separation energy		total energy	
	heating	cooling	heating	cooling
0	0.4	-0.3	0.8	-1.7
1	2.1	-3.1	2.9	-4.3
2	1.1	-2.3	2.5	-5.1
3	1.4	-3.4	2.8	-4.9
4	2.1	-3.2	3.9	-5.3
5	1.9	-2.1	2.6	-3.0
6	2.0	-2.9	3.4	-4.4
7	1.7	-1.8	2.5	-3.2
8	1.7	-3.6	3.9	-7.9
9	1.1	-1.3	2.2	-2.3
10	0.6	-0.8	1.1	-2.6
11	0.5	-0.8	1.5	-1.2
15	3.5	-1.7	3.5	-2.0

a)



b)

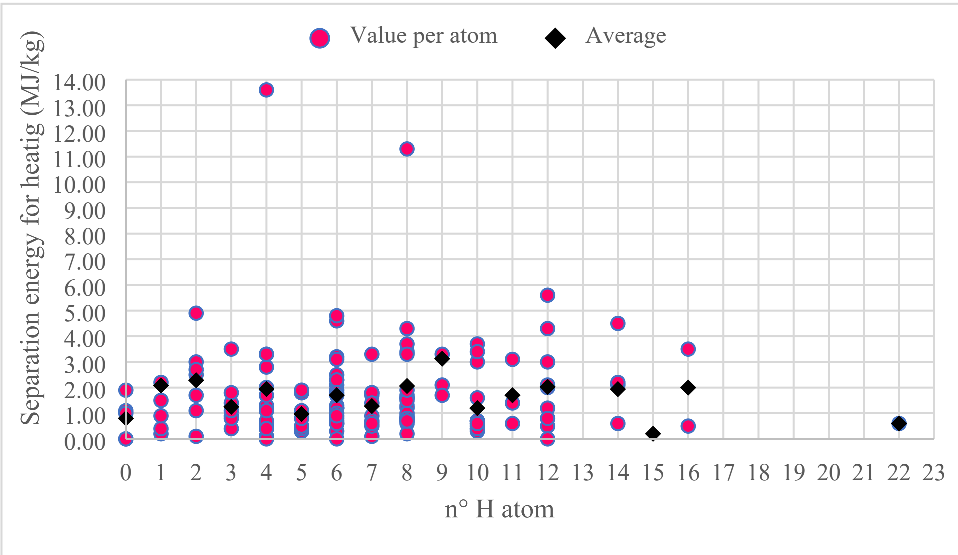
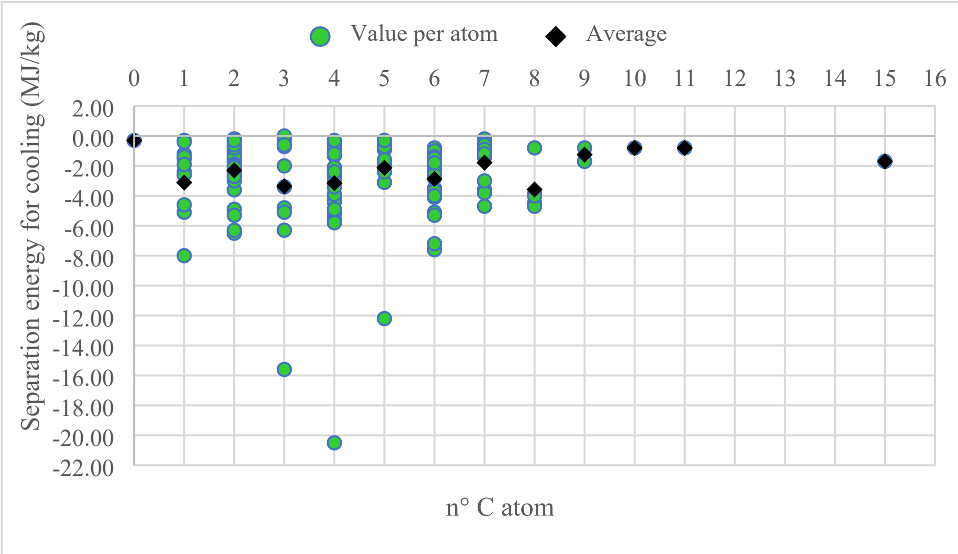


Figure S 1 – Separation energy consumption in MJ/kg for heating procedures plotted per the number of C (a) and H (b) atoms. Data were extrapolated from literature. [20]

a)



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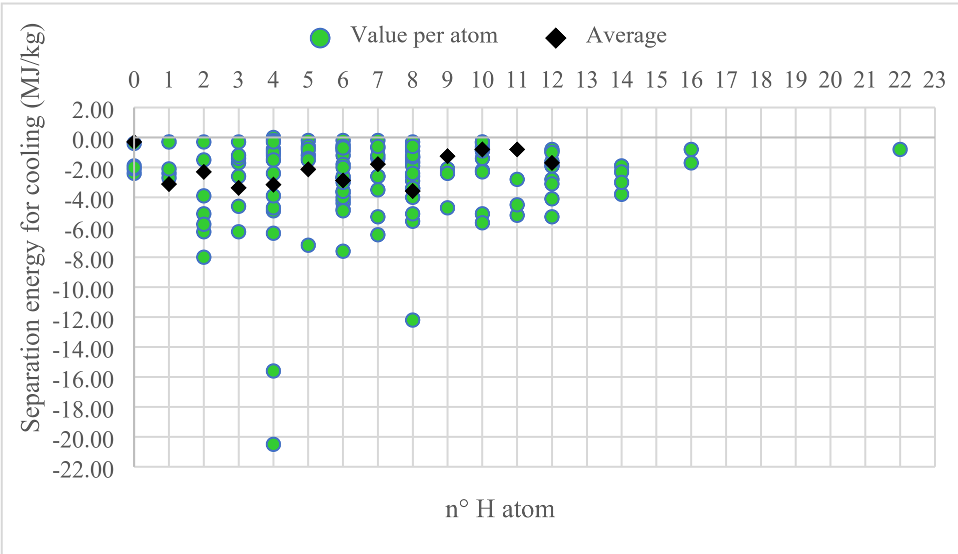

Figure S 2 – Separation energy consumption in MJ/kg for cooling procedures plotted per the number of C (a) and H (b) atoms. Data were extrapolated from literature.[20]

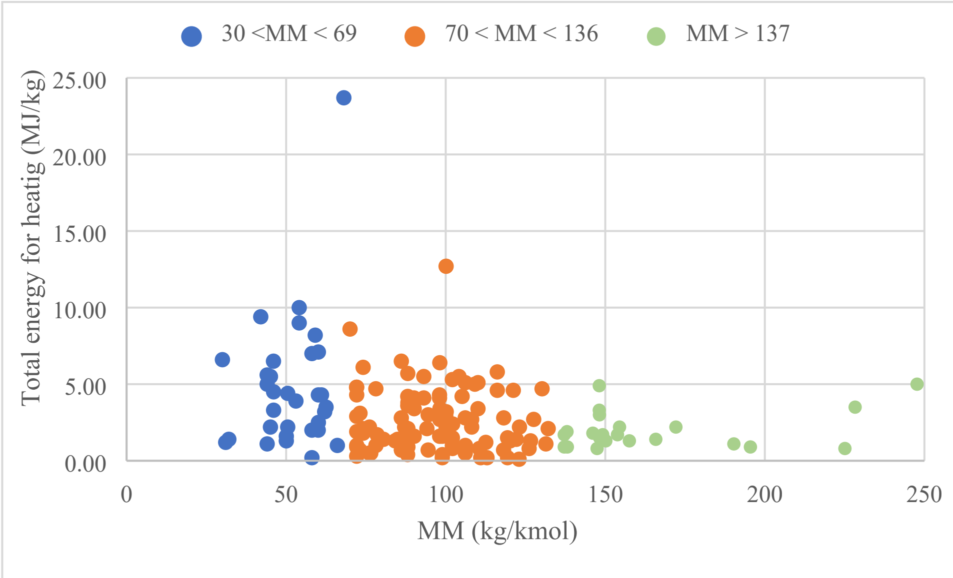

Figure S 3 – Energy for heating (MJ/kg) respect to molecular weight (kg/kmol) subsets: a) 30 < MM < 69, b) 70 < MM < 136, and c) MM >137. Data were extrapolated from literature.[20]

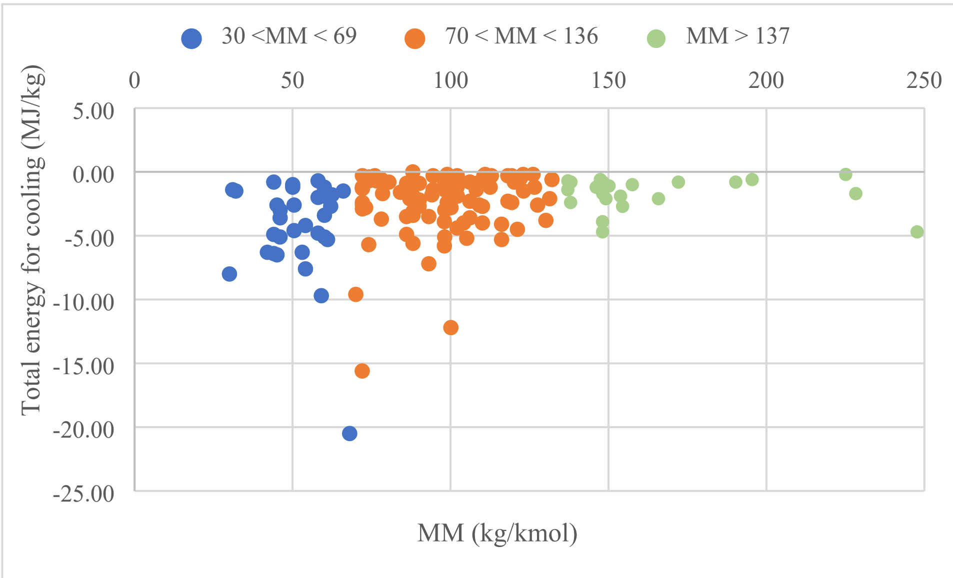

Figure S 4 – Energy for heating (MJ/kg) respect to molecular weight (kg/kmol) subsets: a) 30 < MM < 69, b) 70 < MM < 136, and c) MM >137. Data were extrapolated from literature.[20]

Table S 4 – Mass balance C 100%, S 100%, Y 100%. (1) MO:C1S1Y1 C 100%, S 100%, Y 100%; (4) MA:C1S1Y1 [(1)+Andraos]; (7) MP:C1S1Y1 [(1) + Proxy MA]; (10) MPC:C1S1Y1 [(1) + Proxy C4 avg].

	MM (kg/kmol)	Conversion (%)	Selectivity (%)	Yield (%)	Amount (kg)	Amount (kmol)
Input						
Bio-butanol	74.1	100%	-	-	0.8	1.02E-02
Oxygen (O_2)	32.0	-	-	-	1.3	4.08E-02
Total						5.10E-02
Output						
Maleic anhydride	98.1	-	100.0%	100.0%	1.0	1.02E-02
Water	18.0	-			0.7	4.08E-02
Total						5.10E-02

Table S 5 – Mass balance C 95%, S 100%, Y 95%. (2) MO:C1S1Y0.95 C 95%, S 100%, Y 95%; (5) MA:C1S1Y0.95 [(2)+Andraos]; (8) MP:C1S1Y0.95 [(2) + Proxy MA]; (11) MPC:C1S1Y0.95 [(2) + Proxy C4 avg].

	MM (kg/kmol)	Conversion (%)	Selectivity (%)	Yield (%)	Amount (kg)	Amount (kmol)
Input						
Bio-butanol	74.1	95%	-	-	0.8	1.07E-02
Oxygen (O_2)	32.0	-	-	-	1.3	4.08E-02
Total						5.15E-02
Output						
Maleic anhydride	98.1	-	100.0%	95.0%	1.0	1.02E-02
Water	18.0	-			0.7	4.08E-02
Bio-butanol	74.1				4.0E-02	5.37E-04
Total						5.15E-02

Table S 6 – Mass balance C 100%, S 50%, Y 50%. (3) MO:C1S1Y0.5 C 100%, S 50%, Y 50%; (6) MA:C1S1Y0.5 [(3)+Andraos]; (9) MP:C1S1Y0.5 [(3) + Proxy MA]; (12) MPC:C1S1Y0.5 [(3) + Proxy C4 avg].

	MM (kg/kmol)	Conversion (%)	Selectivity (%)	Yield (%)	Amount (kg)	Amount (kmol)
Input						
Bio-butanol	74.1	100%	-	-	1.5	2.04E-02
Oxygen (O_2)	32.0	-	-	-	2.9	9.18E-02
Total						1.12E-01
Output						
Maleic anhydride	98.1	-	50.0%	50.0%	1.0	1.02E-02
Carbon dioxide	44.0	-	50.0%	50.0%	0.4	1.02E-02

Water	18.0	-	1.7	9.18E-02
Total				1.12E-01

Table S 7 – Energy balance Scen (4) MA:C1S1Y1 [(1)+Andraos] and (5) MA:C1S1Y0.95 [(2)+Andraos], ΔrH° calculation. In the case of MA:C1S1Y0.95 the unreacted butanol does not contribute to the ΔrH°.

Stoichiometric reaction	**$C_4H_{10}O + 3O_2 \rightarrow C_4H_2O_3 + 4H_2O$**	
Input	Δ_fH°r (kJ/mol)	v
Bio-butanol	-274.9	1
Oxigen (O_2)	498.4	3
∑ v❿ΔfH°r	1220.3	
Output	Δ_fH°r (kJ/mol)	v
Maleic anhydride	-398.3	1
Water	-241.8	4
∑ v❿ΔfH°p	-1365.5	
ΔrH°	-2585.8	MJ/kmol
	-7.3	kWh/FU

Table S 8 – Energy balance (6) MA:C1S1Y0.5 [(3)+Andraos], ΔrH° calculation.

Stoichiometric reaction	**$C_4H_{10}O + 9/2O_2 \rightarrow 1/2C_4H_2O_3 + 2\ CO_2 + 9/2H_2O$**	
Input	Δ_fH°r (kJ/mol)	v
Bio-butanol	-274.9	1
Oxigen (O_2)	498.4	4.5
∑ v❿ΔfH°r	1967.9	
Output	Δ_fH°r (kJ/mol)	v
Maleic anhydride	-398.3	0.5
Water	-241.8	4.5
Carbon dioxide	-393.5	2
∑ v❿ΔfH°p	-2074.2	
ΔrH°	-4042.2	MJ/kmol
	-1.1E+01	kWh/FU

Table S 9 – Energy balance, net energy input (nEI) calculation.

		***q* bio-ButOH (liquid → gas)**			
Cp liq (J/mol K)		**A + BT + CT^2 + DT^3 + ET^4**			
Source:*	A	B	C	D	E
bio-ButOH (liquid)	83.877	5.66E-01	-0.0017208	2.28E-06	-
T1(=Tenv)	298	H at T1	3.95E-02	kJ/mol	
T2(=Tb)	391	H at T2	5.51E-02	kJ/mol	
		ΔH	1.57E-02	kJ/mol	
Cp gas (J/mol K)		**A + B[(C/T)/sinh(C/T)]^2+ D[(E/T)/cosh(E/T)]^2**			
Source:*	A	B	C	D	E
bio-ButOH (gas)	8.16E+00	4.10E-01	-2.26E-04	6.04E-08	-6.28E-12

T1(=Tb)	391	H at T1	3.35E-03	kJ/mol		
T2(=Tr)	613	H at T2	5.25E-03	kJ/mol		
		ΔH	1.90E-03	kJ/mol		
ΔH_{vap} (Source**)	43.29	kJ/mol	390.9	K		
q_{tot} bio-ButOH	4.33E+01	kJ/mol				

***q* oxygen (gas)**					
Cp gas (J/mol K)	**A + B[(C/T)/sinh(C/T)]^2+ D[(E/T)/cosh(E/T)]^2**				
	A	B	C	D	E
	29.526	-8.90E-03	3.81E-05	-3.26E-08	8.86E-12
T1(=Tenv)	298	H at T1	8.80E-03	kJ/mol	
T2(=Tr)	613	H at T2	1.81E-02	kJ/mol	
		ΔH	9.30E-03	kJ/mol	

q* tot reaction**				
q_{tot} bio-ButOH + q oxygen	4.33E+01	kJ/mol	4.33E+04	kJ/kmol
			4.42E+02	kJ/FU
			1.22E-01	kWh/FU

Net energy input = *q* tot reaction - ΔrH° Scen (4) and (5)			
Net energy input	-7.2E+00	kWh/FU	Since negative, it was assumed to be recovered as steam for other processes (9.4E+00 kg steam/FU)
Net energy input = *q* tot reaction - ΔrH° Scen (6)			
Net energy input	-1.1E+01	kWh/FU	Since negative, it was assumed to be recovered as steam for other processes (1.5E+01 kg steam/FU)

*Ludwig's Applied Process Design for Chemical and Petrochemical Plants, Volume 1, Fourth Edition, A. Kayode Coker Gulf Professional Publishing is an imprint of Elsevier 30 Corporate Drive, Suite 400, Burlington, MA 01803, USA Linacre House, Jordan Hill, Oxford OX2 8DP, UK 2007 Elsevier Inc.[3]

**National Institute of Standards and Technology (NIST) available at https://webbook.nist.gov/cgi/cbook.cgi?ID=C71363&Mask=4 (accessed 5 August 2024).[4]

***It represents the energy requirements to heat reagents according to literature.[51]

Table S 10 – MA production from bio-butanol, comparison of different scenarios using the method IPCC 2021, GWP100 incl. CO_2 uptake, v.1.01 (kg CO_2 eq.). (1) MO:C1S1Y1 C 100%, S 100%, Y 100%; (2) MO:C1S1Y0.95 C 95%, S 100%, Y 95%; (3) MO:C1S1Y0.5 C 100%, S 50%, Y 50%; (4) MA:C1S1Y1 [(1)+Andraos], (5) MA:C1S1Y0.95 [(2)+Andraos]; (6) MA:C1S1Y0.5 [(3)+Andraos]; (7) MP:C1S1Y1 [(1) + Proxy MA]; (8) MP:C1S1Y0.95 [(2) + Proxy MA]; (9) MP:C1S1Y0.5 [(3) + Proxy MA]; (10) MPC:C1S1Y1 [(1) + Proxy C4 avg]; (11) MPC:C1S1Y0.95 [(2) + Proxy C4 avg]; (12) MPC:C1S1Y0.5 [(3) + Proxy C4 avg].

	MO:C1S 1Y1	MO:C1S 1Y0.95	MO:C1S 1Y0.5	MA:C1S 1Y1	MA:C1S 1Y0.95	MA:C1S 1Y0.5	MP:C1S 1Y1	MP:C1S 1Y0.95	MP:C1S 1Y0.5	MPC:C1 S1Y1	MPC:C1 S1Y0.95	MPC:C1 S1Y0.5	MA_bio ButOH*
biogenic	0.3	0.5	1.0	0.2	0.4	0.9	0.3	0.5	1.1	0.3	0.5	1.1	0.5
CO_2 uptake	-5.9	-6.3	-11.7	-6.0	-6.3	-11.4	-5.9	-6.3	-12.1	-5.9	-6.2	-11.8	-8.6
fossil	1.6	1.7	3.2	-1.0	-1.0	-1.1	5.0	5.1	6.7	2.8	2.9	4.4	0.5
land transformation	-4.1E-03	-4.3E-03	-7.9E-03	-4.4E-03	-4.9E-03	-8.4E-03	-2.9E-03	-3.0E-03	-7.4E-03	-3.8E-03	-4.0E-03	-7.7E-03	0.1
Net	-4.0	-4.1	-7.5	-6.7	-6.9	-11.6	-0.6	-0.7	-4.3	-2.8	-2.9	-6.4	-7.5

SD	1.0	1.1	2.2	1.3	1.3	2.3	1.1	1.1	2.2	1.0	1.1	2.1	2.9

* Cucciniello et al.[42].

Table S 11 – MA production from bio-butanol, comparison of different scenarios using the method CED, v.1.11 (MJ). ((1) MO:C1S1Y1 C 100%, S 100%, Y 100%; (2) MO:C1S1Y0.95 C 95%, S 100%, Y 95%; (3) MO:C1S1Y0.5 C 100%, S 50%, Y 50%; (4) MA:C1S1Y1 [(1)+Andraos], (5) MA:C1S1Y0.95 [(2)+Andraos]; (6) MA:C1S1Y0.5 [(3)+Andraos]; (7) MP:C1S1Y1 [(1) + Proxy MA]; (8) MP:C1S1Y0.95 [(2) + Proxy MA]; (9) MP:C1S1Y0.5 [(3) + Proxy MA]; (10) MPC:C1S1Y1 [(1) + Proxy C4 avg]; (11) MPC:C1S1Y0.95 [(2) + Proxy C4 avg]; (12) MPC:C1S1Y0.5 [(3) + Proxy C4 avg].

	MO:C1S1Y1	**MO:C1S1Y0.95**	**MO:C1S1Y0.5**	**MA:C1S1Y1**	**MA:C1S1Y0.95**	**MA:C1S1Y0.5**	**MP:C1S1Y1**	**MP:C1S1Y0.95**	**MP:C1S1Y0.5**	**MPC:C1S1Y1**	**MPC:C1S1Y0.95**	**MPC:C1S1Y0.5**	**MA_bioButOH***
Non-renewable, biomass	0.2	0.2	0.3	0.2	0.2	0.3	0.2	0.2	0.3	0.2	0.2	0.3	0.2
Non-renewable, nuclear	1.2	1.3	2.5	0.2	0.2	0.7	2.5	2.5	3.7	1.7	1.7	2.9	0.7
Non renewable, fossil	17.3	18.3	34.7	-23.7	-22.9	-30.8	71.2	71.7	88.1	36.0	37.2	53.6	-1.7
Renewable, biomass	63.5	67.0	127.3	63.9	66.9	126.2	64.0	67.9	126.8	64.0	67.9	128.1	92.1
Renewable, water	0.5	0.6	1.1	0.3	0.3	0.7	1.1	1.1	1.6	0.7	0.7	1.3	0.4
Renewable, wind, solar, geothe	0.2	0.2	0.3	0.0	0.0	0.1	0.4	0.4	0.5	0.2	0.2	0.4	0.1
Net	82.9	87.4	166.1	40.8	44.7	97.2	139.4	143.7	221.0	102.7	108.0	186.5	91.9
SD	18.9	21.7	41.0	23.2	24.7	45.8	21.3	22.0	39.7	20.4	20.9	39.7	27.4

* Cucciniello et al.[42].

Table S 12 – MA production from bio-butanol, comparison of different scenarios using the method of different scenarios using the method IPCC 2021, GWP100 incl. CO_2 uptake, v.1.01 (kg CO_2 eq.). (1) MO:C1S1Y1 C 100%, S 100%, Y 100%; (2) MO:C1S1Y0.95 C 95%, S 100%, Y 95%; (3) MO:C1S1Y0.5 C 100%, S 50%, Y 50%; (4) MA:C1S1Y1 [(1)+Andraos], (5) MA:C1S1Y0.95 [(2)+Andraos]; (6) MA:C1S1Y0.5 [(3)+Andraos]; (7) MP:C1S1Y1 [(1) + Proxy MA]; (8) MP:C1S1Y0.95 [(2) + Proxy MA]; (9) MP:C1S1Y0.5 [(3) + Proxy MA]; (10) MPC:C1S1Y1 [(1) + Proxy C4 avg]; (11) MPC:C1S1Y0.95 [(2) + Proxy C4 avg]; (12) MPC:C1S1Y0.5 [(3) + Proxy C4 avg].The table includes the mean, the standard deviation (SD) and the coefficient of variation (CV).

	MO:C1S1Y1			**MO:C1S1Y0.95**			**MO:C1S1Y0.5**			**MA:C1S1Y1**			**MA:C1S1Y0.95**			**MA:C1S1Y0.5**			**MP:C1S1Y1**			**MP:C1S1Y0.95**			**MP:C1S1Y0.5**			**MPC:C1S1Y1**			**MPC:C1S1Y0.95**			**MPC:C1S1Y0.5**		
Unit	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV
biogenic	0.3	0.1	24.1	0.5	0.1	15.9	1.0	0.2	17.3	0.2	0.1	35.1	0.4	0.1	20.8	0.9	0.2	18.6	0.3	0.1	23.3	0.5	0.1	15.2	1.1	0.2	17.0	0.3	0.1	22.0	0.5	0.1	16.5	1.1	0.2	17.1
CO_2 uptake	-5.9	1.5	-24.8	-6.3	1.5	-23.7	-11.7	3.0	-25.9	-6.0	1.5	-25.8	-6.3	1.6	-25.1	-11.4	2.8	-24.1	-5.9	1.5	-26.0	-6.3	1.5	-24.4	-12.1	3.0	-24.9	-5.9	1.4	-23.6	-6.2	1.6	-25.5	-11.8	2.9	-24.9
fossil	1.6	0.4	24.3	1.7	0.4	23.5	3.2	0.8	25.6	-1.0	0.8	-79.9	-1.0	0.8	-83.3	-1.1	1.3	-123.8	5.0	0.5	10.6	5.1	0.5	9.8	6.7	0.9	13.0	2.8	0.4	14.0	2.9	0.4	15.2	4.4	0.8	17.8
land transformation	0.0	0.0	-98.4	0.0	0.0	-99.8	0.0	0.0	-100.9	0.0	0.0	-89.5	0.0	0.0	-87.6	0.0	0.0	-89.7	0.0	0.0	-141.9	0.0	0.0	-146.8	0.0	0.0	-108.8	0.0	0.0	-111.0	0.0	0.0	-109.2	0.0	0.0	-101.9

Table S 13 – MA production from bio-butanol, comparison of different scenarios using the method of different scenarios using the method CED, v.1.11 (MJ). (1) MO:C1S1Y1 C 100%, S 100%, Y 100%; (2) MO:C1S1Y0.95 C 95%, S 100%, Y 95%; (3) MO:C1S1Y0.5 C 100%, S 50%, Y 50%; (4) MA:C1S1Y1 [(1)+Andraos], (5) MA:C1S1Y0.95 [(2)+Andraos]; (6) MA:C1S1Y0.5 [(3)+Andraos]; (7) MP:C1S1Y1 [(1) + Proxy MA]; (8) MP:C1S1Y0.95 [(2) + Proxy MA]; (9) MP:C1S1Y0.5 [(3) + Proxy MA]; (10) MPC:C1S1Y1 [(1) + Proxy C4 avg]; (11) MPC:C1S1Y0.95 [(2) + Proxy C4 avg]; (12) MPC:C1S1Y0.5 [(3) + Proxy C4 avg]. The table includes the mean, the standard deviation (SD) and the coefficient of variation (CV).

	MO:C1S1Y1			**MO:C1S1Y0.95**			**MO:C1S1Y0.5**			**MA:C1S1Y1**			**MA:C1S1Y0.95**			**MA:C1S1Y0.5**			**MP:C1S1Y1**			**MP:C1S1Y0.95**			**MP:C1S1Y0.5**			**MPC:C1S1Y1**			**MPC:C1S1Y0.95**			**MPC:C1S1Y0.5**		
Impact category	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV	Mean	SD	CV
Non-renewable, biomass	0.2	3.6E-02	23.3	0.2	4.1E-02	24.7	0.3	0.1	24.8	0.2	3.7E-02	23.5	0.2	4.2E-02	25.0	0.3	0.1	24.3	0.2	3.8E-02	24.2	0.2	4.0E-02	24.2	0.3	0.1	23.7	0.2	3.8E-02	24.4	0.2	4.0E-02	23.9	0.3	0.1	23.7
Non-renewable, nuclear	1.2	0.4	35.8	1.3	0.5	39.4	2.5	0.9	36.9	0.2	0.4	270.2	0.2	0.5	214.9	0.7	0.8	116.9	2.5	0.8	31.2	2.5	0.8	31.1	3.7	1.2	32.6	1.7	0.5	33.1	1.7	0.6	32.0	2.9	1.0	35.1
Non renewable, fossil	17.3	4.1	23.6	18.3	4.6	25.5	34.7	8.7	25.0	-23.7	12.1	-51.0	-22.9	12.3	-53.7	-30.8	20.5	-66.6	71.2	7.9	11.1	71.7	7.7	10.7	88.1	10.4	11.8	36.0	4.8	13.3	37.2	4.9	13.3	53.6	8.8	16.4
Renewable, biomass	63.5	14.5	22.8	67.0	16.6	24.7	127.3	31.5	24.8	63.9	15.2	23.7	66.9	16.7	25.0	126.2	31.5	25.0	64.0	15.5	24.1	67.9	16.3	24.0	126.8	30.2	23.8	64.0	15.6	24.4	67.9	16.0	23.6	128.1	30.3	23.7
Renewable, water	0.5	0.1	24.6	0.6	0.1	26.6	1.1	0.3	26.0	0.3	0.1	46.3	0.3	0.2	46.0	0.7	0.3	41.8	1.1	0.1	13.2	1.1	0.2	14.2	1.6	0.3	16.8	0.7	0.1	19.5	0.7	0.1	19.3	1.3	0.3	21.7
Renewable, wind, solar, geothe	0.2	3.9E-02	24.4	0.2	0.0	26.3	0.3	0.1	25.7	2.4E-02	5.3E-02	221.0	3.1E-02	0.1	176.1	1.0E-01	1.0E-01	99.7	0.4	4.2E-02	11.7	0.4	4.6E-02	12.6	0.5	0.1	15.6	0.2	4.2E-02	18.3	0.2	4.3E-02	18.0	0.4	0.1	21.0

Table S 14 – Impact per different energetic vector, expressed in kg CO_2 eq/kWh. Method IPCC 2021, GWP100 incl. CO_2 uptake, v.1.01 (kg CO_2 eq.).

Energetic vector	fossil	biogenic	land transformation	CO_2 uptake	Total
Heat, from steam, in chemical industry {RER}| market for heat, from steam, in chemical industry | APOS, U*	4.0E-01	1.1E-02	7.6E-05	-8.0E-03	4.1E-01
Cooling energy {GLO}| market for cooling energy | APOS, U*	2.5E-01	2.2E-03	1.4E-04	-1.8E-03	2.5E-01
Electricity, medium voltage {Europe without Switzerland}| market group for electricity, medium voltage | APOS, U	3.3E-01	6.5E-02	1.4E-03	-2.8E-02	3.7E-01
Electricity, high voltage {ES}| electricity production, solar thermal parabolic trough, 50 MW | APOS, U	5.4E-02	7.9E-04	3.2E-05	-5.4E-04	5.4E-02
Electricity, high voltage {DE}| electricity production, wind, >3MW turbine, onshore | APOS, U	3.4E-02	8.4E-04	9.0E-05	-6.8E-04	3.4E-02

* used in the simulation.

Table S 15 – Impact per different energetic vector, expressed in MJ/kWh. Method CED, v.1.11 (MJ).

Energetic vector	Non renewable, fossil	Non-renewable, nuclear	Non-renewable, biomass	Renewable, biomass	Renewable, wind, solar, geo	Renewable, water	Total
Heat, from steam, in chemical industry {RER}| market for heat, from steam, in chemical industry | APOS, U*	5.8E-01	1.6E-01	6.4E-05	8.8E-02	3.4E-02	3.9E-02	9.1E-01
Cooling energy {GLO}| market for cooling energy | APOS, U*	4.9E-01	1.4E-01	7.7E-05	1.9E-02	4.5E-02	6.6E-02	7.6E-01
Electricity, medium voltage {Europe without Switzerland}| market group for electricity, medium voltage | APOS, U	1.9E+00	3.8E+00	1.1E-03	3.1E-01	7.7E-01	7.7E-01	7.6E+00
Electricity, high voltage {ES}| electricity production, solar thermal parabolic trough, 50 MW | APOS, U	8.8E-02	1.7E-02	3.9E-05	6.0E-03	4.3E-03	9.7E-03	1.2E-01
Electricity, high voltage {DE}| electricity production, wind, >3MW turbine, onshore | APOS, U	1.4E-01	2.8E-02	1.1E-04	8.1E-03	3.9E+00	2.0E-02	4.1E+00

* used in the simulation.