

Life cycle assessment of bio-based ethers and esters: synthesis from waste biomass and application in extraction processes

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Content:

Emission_torch

It contains the calculations for the emissions when the solvent is lost and incinerated in a flare with no energy recovery (Table S1).

GVL_synthesis

It contains the inventory for the synthesis of γ -valerolactone along with assumptions and calculations (Table S2).

EL_synthesis

It contains the inventory for the synthesis of Ethyl lactate along with assumptions and calculations (Table S3).

2-MeTHF_synthesis

It contains the inventory for the synthesis of 2-Methyl tetrahydrofuran along with assumptions and calculations (Table S4).

CPME_synthesis

It contains the inventory for the synthesis of Cyclopentyl methyl ether along with assumptions and calculations (Table S5).

PE_recovery

It contains the inventory for the recovery of low-density polyethylene (LDPE) using different solvents (CPME, 2-MeTHF and cyclohexane - Table S6).

PHB_extraction

It contains the inventory for the extracton of Polyhydroxybutyrate using different solvents (EL, GVL and DMC - Table S7).

Calculation of CO₂ and VOC emission from the torch when burning the following substances:

Table S1. Calculations for the CO₂ and VOC emissions for each solvent.

Substance	Efficiency (%)	Molecular formula	MM (g/mol)	mass loss (kg)	C mass in substance	CO ₂ emissions (kg)	VOC emissions (kg)	Boiling point (°C) at 1 atm	% loss
GVL	0.9999	C ₅ H ₈ O ₂	100.12	1.19E-01	7.16E-02	2.63E-01	1.19E-05	207.5	0.2
EL	0.9999	C ₅ H ₁₀ O ₃	118.13	1.17E-01	5.95E-02	2.18E-01	1.17E-05	154	0.2
DMC	0.9999	C ₃ H ₆ O ₃	90.09	5.62E-01	2.25E-01	8.24E-01	5.62E-05	90.5	1
Cyclohexane	0.9999	C ₆ H ₁₂	84.16	5.24E-01	4.48E-01	1.64E+00	5.24E-05	80.65	1
2-MeTHF	0.9999	C ₅ H ₁₀ O	86.13	5.75E-01	4.01E-01	1.47E+00	5.75E-05	78	1
CPME	0.9999	C ₆ H ₁₂ O	100.16	5.79E-01	4.16E-01	1.53E+00	5.79E-05	106	1
CO₂			44						
C			12						

Table S2. Inventory for the synthesis of γ -Valerolactone.

Process	Flow	Dataset ecoinvent	Input/output	Amount	Unit	Note
Biomass pretreatment	Biomass		input	16.9	kg	
	H ₂ SO ₄	RER: market for sulfuric acid	input	1.7	kg	1 % (w/v) and 1:10 solid-liquid ratio
	Water	RER: market group for tap water	input	169.5	kg	
	Thermal energy	RER: market group for heat, district heating	input	71.6	MJ	121°C x 20'. We do not consider reaction temperature
	NaOH	RER: market for sodium hydroxide, water	input	3.1	kg	1.5 % (w/v) and 1:20 solid-liquid reaction temperature
	Water	RER: market group for tap water	input	209.4	kg	
	Energy (cooling)	GLO: market for cooling energy, at -1°C	input	8.8	MJ	10°C x 1h
	Cellulose	intermediate product	output	6.7	kg	From biomass to cellulose, 39.3 %
	Water recovered		output	375.1	kg	99% is recovered
	Water lost	emission	output	3.8	kg	
Cellulose hydrolysis	Cellulose	intermediate product	input	6.7	kg	
	H ₂ SO ₄	RER: market for sulfuric acid	input	1.1	kg	
	Water	RER: market group for tap water	input	53.4	kg	1:8 solid-liquid ratio
	Thermal energy	RER: market group for heat, district heating	input	30.2	MJ	155°C x 10'
	Glucose	intermediate product	output	4.7	kg	From cellulose to glucose, 71% efficiency
	Water recovered		output	52.8	kg	99% is recovered
	Water lost	emission	output	0.5	kg	
GVL production	D-glucose	intermediate product	input	4.7	kg	0.5 mol/l (Table 2)
	H ₂	RER: market for hydrogen, gaseous, 1 bar	input	0.02	kg	Hydrogen (initial 60 bar at room temperature)
	Thermal energy	RER: market group for heat, district heating	input	34.8	MJ	180°C
	Water	RER: market group for tap water	input	52.0	kg	0.5 mol/l è stata ricircolata l'acqua al 99% mentre l'1% di H ₂ O viene perso e non trattato.
	Energy for distillation	RER: market group for heat, district heating	input	0.5	MJ	T 350-355 °C
	Formic acid	substitution: RER: market for formic acid	output	0.2	kg	16% mol yield
	Water recovered		output	51.5	kg	99% is recovered
	Water lost	emission	output	0.5	kg	
	GVL		output	1.0	kg	38% mol yield. 1kg di GVL = 10 mol

Energy consumption estimate		
Water		
room temperature	20 °C	293.15 K
reaction temperature 1	121 °C	394.15 K
reaction temperature 2	155 °C	428.15 K
reaction temperature 3	10 °C	283.15 K
reaction temperature 4	180 °C	453.15 K
specific heat	4186 J/(kg*K)	
Energy for pretreatment	422786 J/kg	0.42279 MJ/kg
Energy for cooling	41860 J/kg	0.04186 MJ/kg
Energy for hydrolysis	565110 J/kg	0.56511 MJ/kg
Energy for GVL production	669760 J/kg	0.66976 MJ/kg
GVL		
enthalpy of vaporization 2-Me1	53.5 kJ/mol	
Molar Weight	100.12 g/mol	
enthalpy of vaporization (latent)	534358.7695 J/kg	
Energy for distillation	534358.7695 J/kg	0.534359 MJ/kg

Source for glucose production: Dussan K.J., Silva D.D.V., Moraes E.J.C., Arruda P.V., Felipe M.G.A., 2014, Dilute-acid hydrolysis of cellulose to glucose from sugarcane bagasse, *Chemical Engineering Transactions*, 38, 433-438 DOI: 10.3303/CET1438073

Source for GVL production: Hans Heeres, Ratna Handana, Dai Chunai, Carolus Borromeus Rasrendra, Buana Girisuta and Hero Jan Heeres. 2009. Combined dehydration/(transfer)-hydrogenation of C6-sugars (D-glucose and D-fructose) to γ -valerolactone using ruthenium catalysts. *Green Chemistry*. DOI: 10.1039/b904693c

Table S3. Inventory for the synthesis of Ethyl lactate.

Process	Flow	Datasetecoinvent	Input/output	Amount	Unit	Note
Biomass pretreatment	Biomass		input	4.14	kg	
	H ₂ SO ₄	RER: market for sulfuric acid	input	0.41	kg	1 % (w/v) and 1:10 solid-liquid ratio
	Water	RER: market group for tap water	input	41.45	kg	
	Thermal energy	RER: market group for heat, district	input	17.52	MJ	121°C x 20'. We do not consider the energy consumption for heating the biomass
	NaOH	RER: market for sodium hydroxide, v	input	0.77	kg	1.5 % (w/v) and 1:20 solid-liquid ratio. Starting from 10°C
	Water	RER: market group for tap water	input	51.22	kg	
	Energy (cooling)	GLO: market for cooling energy, at -	input	2.14	MJ	10°C x 1h
	Cellulose	intermediate product	output	1.63	kg	From biomass to cellulose, 39.37 % efficiency. Starting from 10°C
	Water recovered		output	91.74	kg	99% is recovered
	Water lost	emission	output	0.93	kg	
Cellulose hydrolysis	Cellulose		input	1.63	kg	
	H ₂ SO ₄	RER: market for sulfuric acid	input	0.26	kg	
	Water	RER: market group for tap water	input	13.05	kg	1:8 solid-liquid ratio
	Thermal energy	RER: market group for heat, district	input	7.38	MJ	155°C x 10'
	Glucose	intermediate product	output	1.16	kg	From cellulose to glucose, 71% efficiency
	Water recovered		output	12.92	kg	99% is recovered
LA extraction	Water lost	emission	output	0.13	kg	
	Glucose	intermediate product	input	1.16	kg	
	Fermentation broth		input	1.65	kg	yield of 92% of lactic acid from fermentation broth could be achieved. But LA is 69% of the fermentation broth
	Calcium hydroxide	RoW: market for hydrated lime, loose	input	0.47	kg	
	Sulfuric acid	RER: market for sulfuric acid	input	0.62	kg	
	Calcium sulfate	RER: market for anhydrite	output	0.86	kg	
Reactive distillation	Lactic acid	intermediate product	output	1.04	kg	most of the lactic acid (98%) had been recovered. molar ratio 3.6:1 (EtOH:LA). Reaction E6 (Table 2 and Table 3)
	Lactic acid	intermediate product	input	1.04	kg	
	Ethanol	RER: ethanol production, ethylene h	input	1.92	kg	
	Energy	RER: market group for heat, district	input	0.47	MJ	95 °C
	Water	RER: treatment of wastewater from	output	0.21	kg	
	Ethyl lactate		output	1.00	kg	total yield 73%

Energy consumption estimate

Water		
room temperature	20 °C	293.15 K
reaction temperature 1	121 °C	394.15 K
reaction temperature 2	155 °C	428.15 K
reaction temperature 3	10 °C	283.15 K
specific heat	4186 J/(kg*K)	
Energy for pretreatment	422786 J/kg	0.42279 MJ/kg
Energy for hydrolysis	565110 J/kg	0.56511 MJ/kg
Energy for cooling	41860 J/kg	0.04186 MJ/kg

Ethanol

room temperature	20 °C	293.15 K
reaction temperature	95 °C	368.15 K
specific heat ¹	111.96 J/(mol*K)	
molar mass	46.07 g/mol	
Energy	182266.1168 J/kg	0.18227 MJ/kg

Lactic acid

room temperature	20 °C	293.15 K
reaction temperature	95 °C	368.15 K
specific heat ²	142.95 J/(mol*K)	
molar mass	90.08 g/mol	
Energy	119019.2052 J/kg	0.11902 MJ/kg

Stoichiometry calculations

LA extraction							
Calcium hydro		Fermentation broth (LA)		lilfuric ac	⇒	LA	cium sulfate
	CaOH ₂	C ₃ H ₆ O ₃	H ₂ SO ₄	⇒		C ₃ H ₅ O ₃	CaSO ₄
g/mol	74.1	90.08	98.08			90.08	136.14
mol	6	12	6			11	6
g	444.6	1080.96	588.48			994.48	816.84
g		447.07	1086.96	591.74		1000	821.37

EL production

	EtOH	LA	⇒	EL	water
	C ₂ H ₆ O	C ₃ H ₆ O ₃	⇒	C ₅ H ₁₀ O ₃	H ₂ O
g/mol	46.07	90.08		118.13	18
mol	3.6	1		0.73	1
g	165.852	90.08	0	86.235	18
g	1923.26	1044.59		1000	208.73

¹ <https://www.chemeo.com/cid/35-653-8/Ethanol>

² <https://www.chemeo.com/cid/21-090-8/Lactic-acid>

Source for glucose production: Dussan K.J., Silva D.D.V., Moraes E.J.C., Arruda P.V., Felipe M.G.A., 2014, Dilute-acid hydrolysis of cellulose to glucose from sugarcane bagasse

Source for LA extraction: Da-Jeong Min, Kook Hwa Choi, Yong Keun Chang, and Jin-Hyun Kim. 2011. Effect of operating parameters on precipitation for recovery of lactic acid

Source for EL production: Navinchandra Asthana, Aspi Kolah, Dung T. Vu, Carl T. Lira, and Dennis J. Miller. 2005. A Continuous Reactive Separation Process for Ethyl Lactate

Table S4. Inventory for the synthesis of 2-Methyl tetrahydrofuran.

Process	Flow	Dataset ecoinvent	Input/output	Amount	Unit	Note
Biomass pretreatment	Biomass		input	32.8	kg	
	H ₂ SO ₄	RER: market for sulfuric acid	input	3.3	kg	1 % (w/v) and 1:10 solid-liquid ratio
	Water	RER: market group for tap water	input	328.4	kg	
	Thermal energy	RER: market group for heat, dist	input	138.8	MJ	121°C x 20'. We do not consider the en
	NaOH	RER: market for sodium hydroxid	input	6.1	kg	1.5 % (w/v) and 1:20 solid-liquid ratio. ‡
	Water	RER: market group for tap water	input	405.8	kg	
	Energy (cooling)	GLO: market for cooling energy,	input	17.0	MJ	10°C x 1 h
	Cellulose	intermediate product	output	12.9	kg	From biomass to cellulose, 39.37 % effi
Cellulose hydrolysis	Water recovered		output	660.8	kg	99% is recovered
	Water lost	emission	output	73.4	kg	
	Cellulose	intermediate product	input	12.9	kg	
	H ₂ SO ₄	RER: market for sulfuric acid	input	2.1	kg	
	Water	RER: market group for tap water	input	103.4	kg	1:8 solid-liquid ratio
	Thermal energy	RER: market group for heat, dist	input	58.5	MJ	155°C x 10'
	Glucose	intermediate product	output	9.2	kg	From cellulose to glucose, 71% efficien
	Water recovered		output	102.4	kg	99% is recovered
GVL production	Water lost	emission	output	1.0	kg	
	D-glucose	intermediate product	input	9.2	kg	0.5 mol/l (Table 2)
	H ₂	RER: market for hydrogen, gase	input	0.04	kg	Hydrogen (initial 60 bar at room tempe
	Thermal energy	RER: market group for heat, dist	input	67.5	MJ	180°C
	Water	RER: market group for tap water	input	100.8	kg	0.5 mol/l è stata ricircolata l'acqua al 99% mentre l'1% di H2O viene perso e non trattato.
	Formic acid	substitution: RER: market for fo	output	0.4	kg	16% mol yield
	Water recovered		output	99.8	kg	99% is recovered
	Water lost	emission	output	1.0	kg	
Hydrogenation	GVL	intermediate product	output	1.9	kg	38% mol yield. 1kg di GVL = 10 mol
	GVL	intermediate product	input	1.9	kg	
	H ₂	RER: market for hydrogen, gase	input	0.1	kg	
	Energy	RER: market group for heat, dist	input	0.4	MJ	160°C
	1,4-PDO	intermediate product	output	2.0	kg	
Dehydration Cyclisation	Energy	RER: market group for heat, dist	input	0.7	MJ	
	Energy for distillation	RER: market group for heat, dist	input	0.4	MJ	
	2MeTHF		output	1.0	kg	60% yield
	H2O	RER: treatment of wastewater fr	output	0.2	kg	

Energy consumption estimate

Water			
room temperature	20 °C	293.15 K	
reaction temperature	121 °C	394.15 K	
reaction temperature	155 °C	428.15 K	
reaction temperature	10 °C	283.15 K	
reaction temperature	180 °C	453.15 K	
specific heat	4186 J/(kg*K)		
Energy for pretreatme	422786 J/kg	0.42279 MJ/kg	
Energy for cooling	41860 J/kg	0.04186 MJ/kg	
Energy for hydrolysis	565110 J/kg	0.56511 MJ/kg	
Eney for GVL produc	669760 J/kg	0.66976 MJ/kg	

GVL			
room temperature	20 °C	293.15 K	
reaction temperature	160 °C	433.15 K	
molar mass	100.12		
specific heat	154.05 J/(mol*K)		
specific heat	1538.65 J/(kg*K)		
Energy	215412 J/kg	0.21541 MJ/kg	

1,4-PDO			
room temperature	20 °C	293.15 K	
reaction temperature	200 °C	473.15 K	
molar mass	104		
specific heat	213.31 J/(mol*K)		
specific heat	2051.06 J/(kg*K)		
Energy	369190 J/kg	0.36919 MJ/kg	

2MeTHF			
enthalpy of vaporizati	33.7 kJ/mol		
molar mass	86.13 g/mol		
entalpia di vaporizzazi	391269 J/kg		
Energy for distillation	3.91E+05 J/kg	0.39 MJ/kg	

Stoichiometry calculations

2MeTHF production						
	GVL	1,4-PDO	2 H ₂	⇒	2MeTHF	H2O
g/mol	100	104	2		86	18
mol	19.38	19.38	38.76		11.63	11.63
kg	1.94	2.02	0.08		1	0.21

Source for glucose production: Dussan K.J., Silva D.D.V., Moraes E.J.C., Arruda P.V., Felipe M.G.A., 2014, Dilute-acid hydrolysis of cellulose to glucose from sugarcane bagasse, Chemical Engineering Transactions, 38, 433-438 DOI: 10.3303/CET1438073

Source for GVL production: Hans Heeres, Ratna Handana, Dai Chunai, Carolus Borromeus Rasrendra, Buana Girsuta and Hero Jan Heeres. 2009. Combined dehydration/(transfer)-hydrogenation of C6-sugars (D-glucose and D-fructose) to c-valerolactone using ruthenium catalysts. Green Chemistry. DOI: 10.1039/b904693c

Source for 2MeTHF production: Qiang Liu, Zhenbo Zhao, Masahiko Arai, Chao Zhang, Ke Liu, Ruhui Shi, Peixuan Wu, Zhuangqing Wang, Weiwei Lin, Haiyang Cheng, Fengyu Zhao, 2020, Transformation of γ-valerolactone into 1,4-pentanediol and 2-methyltetrahydrofuran over Zn-promoted Cu/Al2O3 catalysts. Catal. Sci. Technol., 10, 4412-4423. DOI https://doi.org/10.1039/D0CY00801J & Jiebang Peng, Donghong Zhang, Xin Tian, Mingyue Ding, 2024. Selective hydrogenation of γ-valerolactone to 1,4-pentanediol over hydrotalcite-derived CuCoAl catalysts. https://doi.org/10.1016/j.fuproc.2024.108068

Table S5. inventory for the synthesis of Cyclopentyl methyl ether.

Process	Flow	Datasetecoinvent	Input/output	Amount	Unit
Depolymerization	HFLBa		input	8.50	kg
	NaOH	RER: market for sodium hydroxide,	input	0.50	kg
	H2O	RER: market group for tap water	input	1.00	kg
	Steam	RER: market for steam, in chemical	input	19.25	kg
	Solid fraction	RER: treatment of inert waste, sanit	output	7.00	kg
Fermentation	NaOH	RER: market for sodium hydroxide,	input	1.00	kg
	(NH4)2HPO4	RER: market for diammonium phos	input	0.0005	kg
	Corn steep liqu	not found	input	0.005	kg
	Air	natural resource	input	10.00	kg
	Electricity	RER: market group for electricity, m	input	2.70	MJ
Separation	H2SO4	RER: market for sulfuric acid	input	2.00	kg
	NaOH	RER: market for sodium hydroxide,	input	0.01	kg
	Energy (cooling	GLO: market for cooling energy, at -	input	1.75	MJ
	Electricity tot	RER: market group for electricity, m	input	0.36	MJ
	Fermentation b	RER: treatment of wastewater from	output	19.50	kg
	Na2SO4	RER: market for sodium sulfate, anh	output	2.75	kg
Upgrade	EtOH	RER: ethanol production, ethylene f	input	0.18	kg
	NaOH	RER: market for sodium hydroxide,	input	0.01	kg
	H2SO4	RER: market for sulfuric acid	input	2.00	kg
	H2	RER: market for hydrogen, gaseous,	input	0.08	kg
	Energy (cooling	GLO: market for cooling energy, at -	input	30.00	MJ
	Electricity	RER: market group for electricity, m	input	0.90	MJ
	Thermal energy	RER: market group for heat, district	input	52.50	MJ
From AA to cyclopentanone	AA	intermediate product	output	2.50	kg
	AA	intermediate product	input	2.50	kg
	NaOH	RER: market for sodium hydroxide,	input	0.02	kg
	Thermal energy	RER: market group for heat, district	input	1.50	MJ
	CO2	emission	output	0.70	kg
	Wastewater	RER: treatment of wastewater from	output	0.30	kg
	Humins	intermediate product	output	0.20	kg
From cyclopentanone to cyclopentanol	Cyclopentanone	intermediate product	output	1.30	kg
	Cyclopentanone	intermediate product	input	1.30	kg
	H2O	RER: market group for tap water	input	26.00	kg
	Thermal energy	RER: market group for heat, district	input	0.30	MJ
	Wastewater	RER: treatment of wastewater from	output	26.00	kg
	Humins	intermediate product	output	0.08	kg
	Cyclopentanol	intermediate product	output	1.20	kg
From cyclopentanol to CPME	Cyclopentanol	intermediate product	input	1.20	kg
	MeOH	CH: market for methanol, from bior	input	0.20	kg
	N2 (gas)	RER: market for nitrogen, liquid	input	4.56	kg
	Thermal energy	RER: market group for heat, district	input	0.04	MJ
	Wastewater	RER: treatment of wastewater from	output	0.20	kg
	Cyclopentene	intermediate product	output	0.10	kg
	Humins	intermediate product	output	0.20	kg
	CPME		output	1.00	kg
Humin upgrading	Humins		input	0.50	kg
	Thermal energy	RER: market group for heat, district	output	7.60	MJ

Table S6.1 Inventory for the recovery of LDPE using 2-MeTHF

Process	Flows	Dataset	input/ output		Units	Note
Dissolution (15' + 15')	PolyAl		input	1.35	kg	2% of PolyAl in 60 mL of 2-MeTHF
	2-MeTHF	see 2-MeTHF synt	input	57.51	kg	
	Thermal energy	RER: market grou	input	8.54	MJ	100 °C
	PolyAl + 2-MeTHF	intermediate	output	58.86	kg	
Filtration	PolyAl + 2-MeTHF	intermediate	input	58.86	kg	
	LDPE + 2-MeTHF	intermediate	output	57.93	kg	
	Aluminium	substitution: IAI A	output	0.33	kg	No 2-MeTHF residues on the Al
	VOC (2MeTHF comb.)	emission	output	5.75E-05	kg	Losses to atmosphere
	CO2 (2MeTHF comb.)	emission	output	1.47	kg	
Distillation	LDPE + 2-MeTHF	intermediate	input	57.93	kg	
	Thermal energy	RER: market grou	input	22.47	MJ	
	Recovered 2-MeTHF		output	56.93	kg	2-MeTHF recovery is 99%
	LDPE		output	1.00	kg	No 2-MeTHF residues on the LDPE

Table S6.2 Inventory for the recovery of PE using 2-MeTHF

Process	Flows	Dataset	input/ output		Units	Note
Dissolution (15' + 15')	PolyAl		input	1.35	kg	2% of PolyAl in 60 mL of CPME
	CPME	see CPME synthesis	input	57.91	kg	
	Thermal energy	RER: market group	input	5.99	MJ	100 °C
	PolyAl + CPME	intermediate	output	59.26	kg	
Filtration	PolyAl + CPME	intermediate	input	59.26	kg	
	LDPE + CPME	intermediate	output	58.33	kg	
	Aluminium	substitution: IAI A	output	0.33	kg	No CPME residues
	VOC (CPME comb.)	emission	output	5.79E-05	kg	Losses to atmosphere
	CO2 (CPME comb.)	emission	output	1.53	kg	
Distillation	LDPE + CPME	intermediate	input	58.33	kg	
	Thermal energy	RER: market group	input	16.60	MJ	
	Recovered CPME		output	57.33	kg	CPME recovery is 99%
	LDPE		output	1.00	kg	No CPME residues on the LDPE

Table S6.3 Inventory for the recovery of PE using cyclohexane.

Process	Flows	Dataset	input/output		Units	Note
Dissolution (15' + 15')	PolyAl		input	1.35	kg	2% of PolyAl in 60 mL
	cyclohexane	RER: cyclohexane	input	52.39	kg	
	Thermal energy	RER: market grou	input	7.78	MJ	T = 100 °C
	PolyAl + cyclohexane	intermediate	output	53.74	kg	
Filtration	PolyAl + cyclohexane	intermediate	input	53.74	kg	
	LDPE + cyclohexane	intermediate	output	52.87	kg	
	Aluminium	substitution: IAI A	output	0.33	kg	No cyclohexan residues
	VOC	emission	output	5.24E-05	kg	Losses to atmosphere
	CO2	emission	output	1.64	kg	
Distillation	LDPE + cyclohexane	intermediate	input	52.87	kg	
	Thermal energy	RER: market grou	input	19.10	MJ	
	Recovered cyclohexane		output	51.87	kg	Cyclohexane recovery is 99%
	LDPE		output	1.00	kg	No cyclohexan residues

Energy consumption estimate		
2-MeTHF		
room temperature	20 °C	293.15 K
extraction temperature	100 °C	373.15 K
specific heat	1857 J/(kg*K)	
enthalpy of vaporization 2-MeTHF	34 kJ/mol	
Molar Weight	86.13 g/mol	
enthalpy of vaporization (latent heat)	3.95E+05 J/kg	
Energy for dissolution	1.49E+05 J/kg	0.14856 MJ/kg
Energy for distillation	3.95E+05 J/kg	0.3947521 MJ/kg

CPME		
room temperature	20 °C	285.65 K
extraction temperature	100 °C	343.15 K
specific heat	1799.12 J/(kg*K)	
enthalpy of vaporization (latent heat)	289.5328 J/g	
Energy for dissolution	1.03E+05 J/kg	0.10345 MJ/kg
Energy for distillation	2.90E+05 J/kg	0.28953 MJ/kg

Cyclohexane		
room temperature	20 °C	293.15 K
extraction temperature	100 °C	373.15 K
specific heat	1857 J/(kg*K)	
enthalpy of vaporization	31 kJ/mol	
Molar Weight	84.16 g/mol	
enthalpy of vaporization (latent heat)	368346.0076 J/g	
Energy for dissolution	1.49E+05 J/kg	0.148560 MJ/kg
Energy for distillation	3.68E+05 J/kg	0.368346 MJ/kg

Table S7.1 Inventory for the extracton of PHB using Ethyl lactate

Process	Flusso	Dataset	nput/output	Amount	Unità	Note
PHB extractio n	Bacteria		input	2.84	kg	
	Solvent EL	see EL synth	input	58.61	kg	20mL
	Total energy	RER: market	input	9.14	MJ	110°, 1h
	Bacteria	CH: treatmer	output	1.84	kg	
	PHB		output	1.00	kg	38.50%
	CO2	emission	output	0.22	kg	
	VOC	emission	output	1.17E-05	kg	
	EL recovered		output	58.49	kg	99.8% recovery
	Energy for distillation	RER: market	input	25.88	MJ	

Table S7.2 Inventory for the extracton of PHB using γ -valerolactone

Process	Flusso	Dataset	nput/output	Amount	Unità	Note
PHB extractio n	Bacteria		input	2.84	kg	
	Solvent GVL	see GVL synt	input	59.74	kg	20mL
	Total energy	RER: market	input	8.27	MJ	110°, 1h
	Bacteria	CH: treatmer	output	1.84	kg	
	PHB		output	1.00	kg	34.75%
	CO2	emission	output	0.26	kg	
	VOC	emission	output	1.19E-05	kg	
	GVL recovered		output	59.62	kg	99.8% recovery
	Energy for distillation	RER: market	input	32.22	MJ	

Table S7.3 Inventory for the extracton of PHB using dimethylcarbonate

Process	Flusso	Dataset	nput/output	Amount	Unità	Note
PHB extractio n	Bacteria		input	2.65	kg	
	Solvent DMC	RER: dimethy	input	56.25	kg	20mL
	Total energy	RER: market	input	9.27	MJ	110°, 1h
	Bacteria	CH: treatmer	output	1.65	kg	
	PHB		output	1.00	kg	35.68%
	CO2	emission	output	0.82	kg	
	VOC	emission	output	5.62E-05	kg	
	DMC recovered		output	55.69	kg	99% recovery
	Energy for distillation	RER: market	input	23.73	MJ	

Energy consumption estimate

EL

room temperature	20 °C	293.15 K
reaction temperatur	110 °C	383.15 K
specific heat1	204.8 J/(mol*K)	
molar mass	118.13 g/mol	
enthalpy of vaporiza	52.17 kJ/mol	
Energy	156031.4907 J/kg	0.15603 MJ/kg
Energy for distillatio	441632.1002 J/kg	0.44163 MJ/kg

GVL

room temperature	20 °C	293.15 K
reaction temperatur	110 °C	383.15 K
specific heat2	154.05 J/(mol*K)	
molar mass	100.12 g/mol	
enthalpy of vaporiza	54 kJ/mol	
Energy	138478.8254 J/kg	0.13848 MJ/kg
Energy for distillatio	539352.7767 J/kg	0.53935 MJ/kg

DMC

room temperature	20 °C	293.15 K
reaction temperatur	110 °C	383.15 K
specific heat3	165.02 J/(mol*K)	
molar mass	90.09 g/mol	
enthalpy of vaporiza	38 kJ/mol	
Energy	164855.1449 J/kg	0.16486 MJ/kg
Energy for distillatio	421800.4218 J/kg	0.42180 MJ/kg

1 <https://www.chemeo.com/cid/60-712-4/Propanoic-acid-2-hydroxy-ethyl-ester>2 <https://www.chemeo.com/cid/35-335-1/2-3H-Furanone-dihydro-5-methyl>3 https://www.chemeo.com/cid/32-123-9/Carbonic-acid-dimethyl-ester#ref-doi_10.1016_j.tca.2004.11.022