Supporting information: Life cycle assessment of adipic acid production from lignin

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S1. Adipic Acid Conventional Production

Adipic acid is a white crystalline solid used in the production of polymeric fibres, plastics, elastomers and lubricants. Commercially, it is the most used aliphatic dicarboxylic acids.[1] Major utilization of adipic acid is in the nylon 6,6 production. It accounts for approximately 90% of the adipic acid demand.[1] Global adipic acid production in 2010 was approximately 3 million tons,[1] mainly in the United States (30%), the European Union (29%), and China (22%).[2] The number of plant producing adipic acid is limited (<30 worldwide**).**[3] **Figure S.1** show the worldwide adipic acid production capacity in 2010.

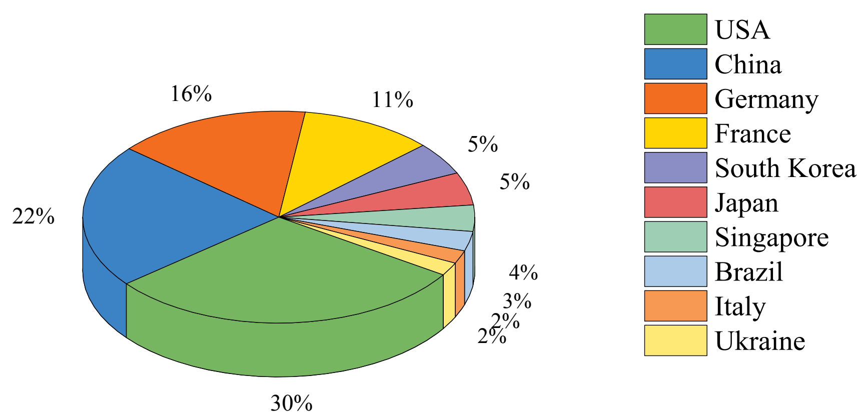

Figure S1. Adipic acid production capacity in 2010.[2]

The current industrial process for adipic acid production is a two-steps reaction that uses cyclohexane, nitric acid and air. Cyclohexane is produced by hydrogenation of benzene using Nickel-based or homogeneous catalyst.[4] In the first step cyclohexane is oxidized with air to produce a mixture of cyclohexanol $(CH_2)_5CHOH$, and cyclohexanone $(CH_2)_5CO$, the mixture is commonly called KA oil. In the second step, the KA oil is oxidized by nitric acid to adipic acid (see **Eq.S1**).[4] In this last reaction NO, NO_2 and N_2O are produced as by-products from HNO_3. Some HNO_3 can be recycled from NO and NO_2. N_2O cannot be recovered and is emitted instead. Stoichiometric emission factor for N_2O production is 0.3 $kg_{N2O}/kg_{adipic\ acid}$.

Eq.S1: $(CH_2)_5CO+(CH_2)_5CHOH+wHNO_3 \rightarrow HOOC(CH_2)_4COOH+xN_2O+yH_2O$

Since 1990, N_2O was recognized as a strong greenhouse gas (GHG factor is 298 kg_{CO2}/kg_{N2O})[5] and several emission reduction strategies were put in place to reduce its emissions from industrial processes.[3] Currently, the most applied emission-abatement strategy is thermal destruction.[3] Thermal destruction is the combustion of off-gases in the presence of methane. Thermal destruction converts N_2O to primarily NO.[5] Thermal destruction allows a reduction up to 97%-99% of the total N_2O emission and currently is the most effective technology on reducing the N_2O emission from the adipic acid and the nitric acid production process. However, N_2O removal is applied in US and Europe; while around 15% of the global production comes from plant without any emission abatement, mainly from China and Ukraine.[2] **Figure S.2** shows the total world adipic acid production capacity in year with or without N2O abatement technology.

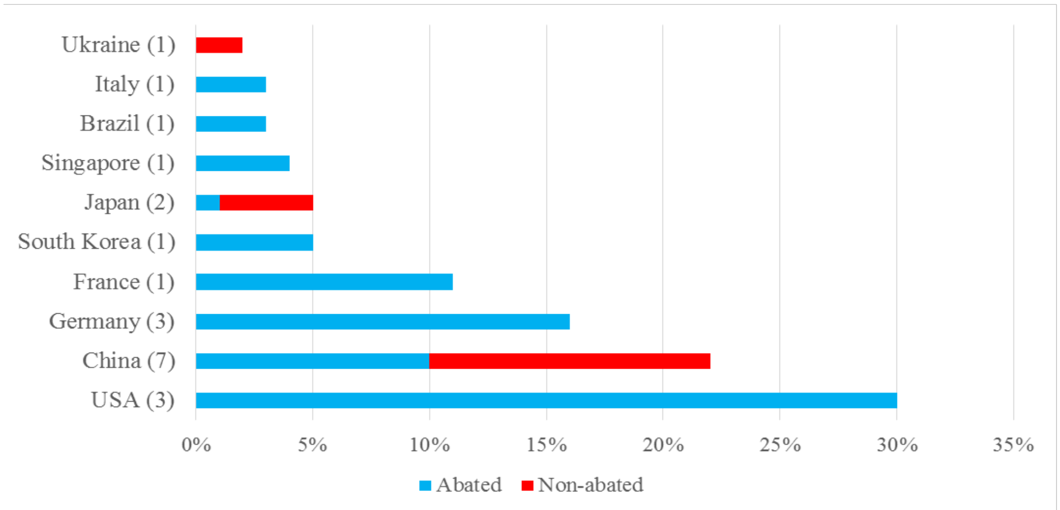

Figure S2. Global share of adipic acid production. The figure shows the global share of adipic acid production plant with or without N_2O abatement technology per country. The number in parenthesis indicates the number of adic acid plants in the specific country. [2]

In the current study two different scenario for conventional adipic acid were developed: CONV-AA-US representing a modern plant with the highest N_2O abatement capacity of 97% and CONV-AA-AVG representing an "average" plant with the world average abatement technology capacity of 85%. In order to evaluate the emission occurred in the two scenario the IPCC emission factor were used.[6,7] To estimate the emission of N_2O due to adipic acid production the following equation S.2 was used:

Eq.S.2: $E_{N2O} = \sum(EF_i * AAP_i'(1 - DF_j * UF_j)$

Where:
E_{N2O}: Emission of nitrous oxide [kg]
EF_i= N_2O emission factor for technology type i [kg N_2O/metric ton of adipic acid]
AAP_i= adipic acid production from technology type i [ton]
DF_j=destruction factor for abatement technology type j [%]
UF_j= utilization factor for abatement technology type j [%]

Table S1. Abatement technology parameters used to estimate the non-abated N2O emission.

Scenario name	Destruction Factor (DF_j)	Utilization factor (UF_j)
CONV-AA-US	98.5%[1]	97%[1]
CONV-AA-AVG	98.5%[1]	85%[2]

[1] From [5]
[2] Calculated based on the world abatement capacity (see Fig S.2)

S2. Lignin conversion process

In the following tables, parameters used for the conversion process in the Aspen models are presented. **Table S2** shows the composition of the high fermentation lignin byproduct (HFLB) originated in the bioethanol biorefinery. **Table S3-S6** present the properties and parameters used in the Aspen model. All the parameters are normalized on a unitary output.

Table S2. HFLB properties and composition.[8]

Component (Aspen name)	Unit	Value
H2O	Kg/h	12796.8
ETHANOL	Kg/h	5.691
GLUCOSE	Kg/h	19.407
GALACTOS	Kg/h	42.601
MANNOSE	Kg/h	17.875
XYLOSE	Kg/h	39.537
ARABINOS	Kg/h	8.193
CELLOB	Kg/h	12.327
GLUCOLIG	Kg/h	42.189
GALAOLIG	Kg/h	1.065
MANOLIG	Kg/h	0.447
XYLOLIG	Kg/h	14.541
ARABOLIG	Kg/h	1.772
EXTRACT	Kg/h	454.535
LGNSOL	Kg/h	24.442
HMF	Kg/h	13.727
FURFURAL	Kg/h	5.455
LACID	Kg/h	63.072
XYLITOL	Kg/h	28.108
GLYCEROL	Kg/h	6.492
SUCCACID	Kg/h	17.041
NH4SO4	Kg/h	92.392
NH4ACET	Kg/h	69.287
DAP	Kg/h	4.797
OIL	Kg/h	0.497
O2	Kg/h	0.535
N2	Kg/h	0.954
CELLULOS	Kg/h	1229.549
GALACTAN	Kg/h	30.36
MANNAN	Kg/h	12.738
XYLAN	Kg/h	414.638
ARABINAN	Kg/h	50.529
LIGNIN	Kg/h	12225.69
PROTEIN	Kg/h	2808.791
ASH	Kg/h	4025.691
ENZYME	Kg/h	510.387
DENZ	Kg/h	56.71
ZYMO	Kg/h	819.265
TRICHO	Kg/h	105.646
TAR	Kg/h	463.634
Properties		
Dry Matter	%wt	62%
LHV	MJ/kg	11.59

Table S3. BCD process details and parameters computed in the Aspen model.

Parameter	Unit	Value
Temperature	°C	160
Pressure	Bar	3.3
HFLB input	kg/kg_{out}	0.379
MP steam input (232°C 9.5atm)	kg/kg_{out}	0.862
Water input	kg/kg_{out}	0.047
NaOH load	%wt bulk	2%
Electricity consumption	kWh/kg_{out}	0.0142
Decontruction rate (total solid)	%	70%
Decontruction rate (lignin)	%	94%
Deconstruction rate (sugars)	%	92%
Solid residue	kg/kg_{out}	0.313
DM solid residue	%	32%
LHV Solid residue	MJ/kg	4.00

Table S4. Composition and calorific value of the solid residue after BCD process.

Component (Aspen name)	Unit	Value
WATER	%wt	67.95%
CELLULOS	%dm	1.02%
GALACTAN	%dm	0.03%
MANNAN	%dm	0.01%
XYLAN	%dm	0.34%
ARABINAN	%dm	0.04%
LIGNIN	%dm	7.59%
PROTEIN	%dm	29.07%
ASH	%dm	41.66%
ENZYME	%dm	5.28%
DENZ	%dm	0.59%
ZYMO	%dm	8.48%
TRICHO	%dm	1.09%
TAR	%dm	4.80%
CELLULOS	%dm	1.02%
Properties		
LHV	MJ/kg	4.00

Table S5. Composition of the liquid residue after BCD process.

Component (Aspen name)	Unit	Value
WATER	%wt	82.72%
ETHANOL	%wt	0.01%
GLUCOSE	%wt	1.32%
GALACTOS	%wt	0.08%
MANNOSE	%wt	0.03%
XYLOSE	%wt	0.49%
ARABINOS	%wt	0.06%
CELLOB	%wt	0.01%
GLUCOLIG	%wt	0.04%
GALAOLIG	%wt	0.00%
MANOLIG	%wt	0.00%
XYLOLIG	%wt	0.02%
ARABOLIG	%wt	0.00%
EXTRACT	%wt	0.47%
LGNSOL	%wt	11.95%
HMF	%wt	0.01%
FURFURAL	%wt	0.01%
LACID	%wt	0.07%
XYLITOL	%wt	0.03%
GLYCEROL	%wt	0.01%
SUCCACID	%wt	0.02%
NH4SO4	%wt	0.10%
NH4ACET	%wt	0.07%
DAP	%wt	0.00%
NAOH	%wt	2.48%
OIL	%wt	0.00%
O2	%wt	0.00%
N2	%wt	0.00%

Table S6. Fermentation process details and parameters computed in the Aspen model.

Parameter	Unit	Value
Temperature	°C	32
Pressure	Bar	1
Deconstructed HFLB input	kg/kg_{out}	1.032
Diammonium Phosphate (DAP)	kg/kg_{out}	2.56E-5
Corn steep liquor (CSL)	kg/kg_{out}	2.73E-4
NaOH (neutralizing agent)	kg/kg_{out}	4.18E-2
Electricity input	kWh/kg_{out}	0.034
Metabolic Yield	%mol	97%
Titer	g/L	80
Fermentation time	h	80
Sodium Muconate production	kg/kg_{out}	0.151

Table S7. Separation process details and parameters computed in the Aspen model.

Parameter	Unit	Value
Temperature	°C	30
Pressure	Bar	1
Fermentation Broth	kg/kg_{out}	8.87E+00
H_2SO_4	kg/kg_{out}	7.93E-01
NaOH	kg/kg_{out}	4.46E-03
Electricity input	kWh/kg_{out}	4.03E-02
Cooling duties	MJ/ kg_{out}	7.54E-01
Na_2SO_4 residue to landfill	Kg/kg_{out}	1.15E+00
Liquid residue to WWT	Kg/kg_{out}	7.52E+00

Table S8. Catalytic upgrading process details and parameters computed in the Aspen model.

Parameter	Unit	Value
Temperature	°C	75
Pressure	Bar	33
Muconic acid	kg/kg_{out}	9.73E-01
Ethanol	kg/kg_{out}	8.75E+00
Hydrogen	kg/kg_{out}	5.52E-02
Ethanol recycling	kWh/kg_{out}	99.23%
Hydrogen recycling	MJ/ kg_{out}	51.66%
Electricity	Kg/kg_{out}	8.67E-02
Heat	MJ/kg_{out}	2.06E+01
Cooling	MJ/kg_{out}	2.34E+00
Conversion efficiency	%	100%

S3: Life Cycle inventory

Table S9. Life Cycle Inventory for the production of 1 kg of adipic acid.

	Component	Unit	Total	Feedstock	BCD	Fermentation	Separation	Upgrade
Material	HFLB	kg	3.37E+00		3.37E+00			
	NaOH	kg	5.85E-01		2.21E-01	3.60E-01	4.34E-03	4.34E-03
	Water	kg	4.17E-01		4.17E-01			
	Air	kg	4.03E+00			4.03E+00		
	Diammonium Phosphate	kg	2.20E-04			2.20E-04		
	Corn steep liquor	kg	2.35E-03			2.35E-03		
	H_2SO_4	kg	7.72E-01				7.72E-01	7.72E-01
	Ethanol makeup	kg	6.74E-02					6.74E-02
	H2 makeup	kg	2.85E-02					2.85E-02
	Catalyst Rh/C	kg	1.10E-05					1.10E-05
Waste	Solid to boiler	kg	2.78E+00		2.78E+00			
	Residue to WWT	kg	7.93E+00				7.76E+00	
	Salt to landfill	kg					1.12E+00	
Energy	Heat	MJ	2.06E+01					2.06E+01
	Steam	kg	7.67E+00		7.67E+00			
	Cooling	MJ	1.18E+01				7.34E-01	1.18E+01
	Electricity	kWh	5.45E-01			2.93E-01	3.92E-02	1.26E-01

Table S10. Inventory for related to the utilization of 1kg of HFLB. The inventory is calculated as the difference between the utilization of the HFLB minus the solid residue after the BCD process.

Output	Amount	Unit	EcoInvent process	Ref
1) HFLB	1.000	kg		
Output/Avoided				
Lime	1.23E-02		Lime {GLO}| market for | Conseq, U	5
Input from Technosphere, Energy and Materials				
Heat	4.730	MJ	ADAPT_NREL_HEAT	5
Electricity	0.424	Kwh	Electricity, medium voltage {MRO, US only}|Market for | Consequential, U	5
Output Emission to Air				
PM (filterable)	-1.99E-05	kg		6
PM10	-1.84E-05	kg		6
PM2.5	-1.59E-05	kg		6
PM (condensible)	-6.05E-07	kg		6
SO2	-1.11E-04	kg		6
NOx	-3.53E-04	kg		6
CO_{bio}	-1.64E-03	kg		6
VOC	-6.05E-05	kg		6
CH_{4bio}	-7.48E-05	kg		6
N2O	-4.63E-05	kg		6
Sulfuric Acid Mist (H_2SO_4)	-1.40E-05	kg		6
Ammonia (NH_3)	-1.50E-07	kg		6
Acetaldehyde	-2.96E-06	kg		6
Acetophenone	-1.14E-11	kg		6
Acrolein	-1.42E-05	kg		6
Antimony & Compounds	-2.81E-08	kg		6
Arsenic & Compounds	-3.92E-08	kg		6
Benzene	-1.50E-05	kg		6
Benzo(a)pyrene	-9.26E-09	kg		6
Beryllium metal (un-reacted)	-1.70E-10	kg		6
Cadmium Metal (elemental un-reacted)	-4.10E-09	kg		6
Carbon tetrachloride	-1.60E-07	kg		6
Chlorine	-2.81E-06	kg		6
Chlorobenzene	-1.18E-07	kg		6
Chloroform	-9.97E-08	kg		6
Chromium–Other compounds	-1.13E-08	kg		6
Cobalt compounds	-2.31E-08	kg		6
Dinitrophenol, 2,4-	-6.41E-10	kg		6
Di(2-ethylhexyl)phthalate (DEHP)	-1.67E-10	kg		6
Ethyl benzene	-1.10E-07	kg		6
Ethylene dichloride (1,2-dichloroethane)	-1.03E-07	kg		6
Formaldehyde	-1.57E-05	kg		6
Hydrogen chloride (hydrochloric acid)	-5.27E-06	kg		6
Hydrogen flouride	-4.70E-07	kg		6
Lead	-1.71E-07	kg		6
Manganese & compounds	-2.73E-08	kg		6
Mercury, vapor	-6.16E-09	kg		6
Methyl bromide (bromomethane)	-5.34E-08	kg		6
Methyl chloride (chloromethane)	-8.19E-08	kg		6
Methyl chloroform (1,1,1 trichloroethane)	-1.10E-07	kg		6
Methylene chloride (dichloromethane)	-1.03E-06	kg		6
Naphthalene	-3.45E-07	kg		6
Nickel metal (Component of Nickel & Compounds)	-6.80E-09	kg		6
Pentachlorophenol	-1.82E-10	kg		6
Phenol	-1.82E-07	kg		6
Phosphorus Metal, Yellow or White	-9.62E-08	kg		6
Polychlorinated biphenyls	-2.90E-11	kg		6
Polycyclic Organic Matter	-4.45E-07	kg		6
Propionaldehyde	-2.17E-07	kg		6
Propylene dichloride (1,2 dichloropropane)	-1.18E-07	kg		6
Selenium compounds	-1.79E-08	kg		6
Styrene	-6.77E-06	kg		6
Tetrachlorodibenzo-p-dioxin, 2,3,7,8-	-3.06E-14	kg		6
Toluene	-3.28E-06	kg		6
Trichloroethylene	-1.07E-07	kg		6

Trichlorophenol, 2,4,6-	-7.83E-11	kg		6
Vinyl chloride	-6.41E-08	kg		6
Xylene, o-	-8.90E-08	kg		6
Waste and Emission to treatment				
Ash+baghouse	-1.64E-02	kg	Wood ash mixture, pure {RoW} | treatment of, sanitary landfill | Conseq, U	6

S4: Additional LCA result not presented in the manuscript

Table S11. Midpoint results for the biobased adipic acid produced in US, biobased adipic acid produced in Denmark, conventional adipic acid produced in US and conventional adipic acid with world average N2O capture potential.

Impact category	Unit	BIO-AA-US	CONV-AA-AVG	CONV-AA-US	BIO-AA-DK
Ozone depletion	Kg $CFC_{11\text{-eq}}$	-1.11E-08	7.39E-07	7.38E-07	9.51E-09
GHG emissions	Kg $CO_{2\text{-eq}}$	4.87E+00	2.26E+01	1.29E+01	4.27E+00
Smog	Kg $O_{3\text{-eq}}$	1.31E-01	1.02E+00	1.00E+00	1.17E-01
Acidification	Kg $SO_{2\text{-eq}}$	2.87E-02	6.18E-02	6.03E-02	1.83E-02
Eutrophication	Kg $N_{\text{-eq}}$	3.64E-03	4.54E-03	5.24E-03	3.17E-03
Carcinogenics	CTU_h	2.72E-08	3.65E-08	3.79E-08	2.40E-08
Non carcinogenics	CTU_h	3.59E-07	3.70E-07	3.79E-07	3.07E-07
Respiratory effects	Kg $PM_{2.5}$	6.56E-03	1.07E-03	2.95E-03	4.55E-03
Ecotoxicity	CTU_e	2.52E+00	3.18E+00	3.18E+00	1.31E+00
Fossil fuel depletion	Kg $CFC_{11\text{-eq}}$	1.38E+01	1.73E+01	1.71E+01	1.45E+01

Table S12. Detailed results of the CONV-AA-US acid scenario. Each scenario has been divided to show the specific contribution of the feedstock materials, production process and the un-abated emission.

Impact category	Unit	Total	Unabated emission	Cyclohexane	Nitric acid	Production process
Ozone depletion	Kg $CFC_{11\text{-eq}}$	7.38E-07	0.00E+00	9.56E-09	2.39E-07	4.90E-07
GHG emissions	Kg $CO_{2\text{-eq}}$	1.29E+01	3.58E+00	1.33E+00	4.63E+00	3.31E+00
Smog	Kg $O_{3\text{-eq}}$	1.00E+00	6.69E-01	5.28E-02	2.10E-01	6.92E-02
Acidification	Kg $SO_{2\text{-eq}}$	6.03E-02	2.89E-02	4.40E-03	1.70E-02	1.00E-02
Eutrophication	Kg $N_{\text{-eq}}$	5.24E-03	1.85E-03	4.93E-04	1.97E-03	9.32E-04
Carcinogenics	CTU_h	3.79E-08	0.00E+00	1.40E-08	1.25E-08	1.14E-08
Non carcinogenics	CTU_h	3.79E-07	0.00E+00	3.32E-08	1.30E-07	2.16E-07
Respiratory effects	Kg $PM_{2.5}$	2.95E-03	0.00E+00	4.52E-04	1.43E-03	1.07E-03
Ecotoxicity	CTU_e	3.18E+00	0.00E+00	5.14E-01	1.58E+00	1.09E+00
Fossil fuel depletion	Kg $CFC_{11\text{-eq}}$	1.71E+01	0.00E+00	6.72E+00	2.68E+00	7.73E+00

Table S13. Detailed results of the CONV-AA-AVG acid scenario. Each scenario has been divided to show the specific contribution of the feedstock amterials, production process and the un-abated emission.

Impact category	Unit	Total	Unabated emission	Cyclohexane	Nitric acid	Production process
Ozone depletion	Kg $CFC_{11\text{-eq}}$	7.39E-07	0.00E+00	9.58E-09	2.39E-07	4.91E-07
GHG emissions	Kg $CO_{2\text{-eq}}$	2.26E+01	1.34E+01	1.33E+00	4.63E+00	3.25E+00
Smog	Kg $O_{3\text{-eq}}$	1.13E+00	7.80E-01	5.31E-02	2.10E-01	8.77E-02
Acidification	Kg $SO_{2\text{-eq}}$	6.66E-02	3.36E-02	4.42E-03	1.70E-02	1.16E-02
Eutrophication	Kg $N_{\text{-eq}}$	4.84E-03	2.16E-03	4.82E-04	1.97E-03	2.39E-04
Carcinogenics	CTU_h	3.66E-08	0.00E+00	1.40E-08	1.25E-08	1.02E-08
Non carcinogenics	CTU_h	3.70E-07	0.00E+00	3.30E-08	1.30E-07	2.07E-07
Respiratory effects	Kg $PM_{2.5}$	1.07E-03	0.00E+00	4.21E-04	1.43E-03	-7.78E-04
Ecotoxicity	CTU_e	3.19E+00	0.00E+00	5.14E-01	1.58E+00	1.10E+00
Fossil fuel depletion	Kg $CFC_{11\text{-eq}}$	1.73E+01	0.00E+00	6.72E+00	2.68E+00	7.90E+00

Table S14. Detailed LCIA midpoint results of the feedstock impacts. The table show the contribution of each input and output on the total score of the process.

Impact category	Unit	Total	CHP natural gas	Avoided lignin combustion	Avoided ash disposal	Avoided lime FGD
Ozone depletion	Kg $CFC_{11\text{-eq}}$	-1.28E-07	4.57E-08	-1.74E-07	-6.86E-11	-3.37E-11
GHG emissions	Kg $CO_{2\text{-eq}}$	4.37E-01	4.53E-01	-1.57E-02	-2.89E-04	-3.83E-04
Smog	Kg $O_{3\text{-eq}}$	-3.97E-03	5.42E-03	-9.33E-03	-3.36E-05	-3.12E-05
Acidification	Kg $SO_{2\text{-eq}}$	8.39E-04	1.22E-03	-3.73E-04	-2.66E-06	-2.39E-06
Eutrophication	Kg $N_{\text{-eq}}$	8.98E-06	2.64E-05	-1.57E-05	-1.38E-06	-3.53E-07
Carcinogenics	CTU_h	4.67E-10	8.11E-10	-3.29E-10	-1.28E-11	-2.72E-12
Non carcinogenics	CTU_h	-1.07E-08	6.69E-09	-1.73E-08	-6.73E-11	-4.45E-11
Respiratory effects	Kg $PM_{2.5}$	7.21E-05	1.04E-04	-3.00E-05	-4.60E-07	-1.21E-06
Ecotoxicity	CTU_e	1.34E-01	1.40E-01	-4.49E-03	-1.25E-03	-1.85E-04
Fossil fuel depletion	MJ surplus	1.12E+00	1.12E+00	0	-6.33E-04	-3.96E-04

Table S15. Detailed LCIA midpoint results of the BCD process. The table show the contribution of each input and output on the total score of the process.

Impact category	Unit	Total	NaOH	Steam	Tap Water	Electricity
Ozone depletion	Kg CFC_{11-eq}	1.73E-08	1.45E-09	1.52E-08	2.97E-12	7.23E-10
GHG emissions	Kg CO_{2-eq}	1.99E-01	3.84E-02	1.51E-01	4.77E-05	9.39E-03
Smog	Kg O_{3-eq}	4.66E-03	2.58E-03	1.84E-03	2.84E-06	2.44E-04
Acidification	Kg SO_{2-eq}	8.14E-04	3.77E-04	4.06E-04	2.48E-07	3.04E-05
Eutrophication	Kg N_{-eq}	1.12E-04	9.26E-05	9.19E-06	2.67E-08	1.05E-05
Carcinogenics	CTU_h	7.34E-10	3.89E-10	3.09E-10	2.08E-12	3.38E-11
Non carcinogenics	CTU_h	1.36E-08	1.08E-08	2.40E-09	9.62E-12	4.16E-10
Respiratory effects	Kg $PM_{2.5}$	2.21E-04	1.50E-04	3.56E-05	9.01E-08	3.54E-05
Ecotoxicity	CTU_e	6.97E-02	2.12E-02	4.71E-02	5.29E-05	1.32E-03
Fossil fuel depletion	MJ surplus	3.86E-01	1.02E-02	3.72E-01	4.61E-05	3.25E-03

Table S16. Detailed LCIA midpoint results of the fermentation process. The table show the contribution of each input and output on the total score of the process.

Impact category	Unit	Total	Diammonium phosphate	Corn steep liquor	Sodium hydroxide	Electricity
Ozone depletion	Kg CFC_{11-eq}	4.07E-09	9.62E-12	0.00E+00	2.43E-09	1.63E-09
GHG emissions	Kg CO_{2-eq}	8.58E-02	5.82E-05	2.45E-06	6.46E-02	2.12E-02
Smog	Kg O_{3-eq}	4.88E-03	3.93E-06	2.02E-07	4.33E-03	5.49E-04
Acidification	Kg SO_{2-eq}	7.04E-04	7.44E-07	2.31E-06	6.33E-04	6.84E-05
Eutrophication	Kg N_{-eq}	1.80E-04	3.74E-07	3.89E-08	1.56E-04	2.36E-05
Carcinogenics	CTU_h	7.33E-10	3.88E-12	3.67E-16	6.53E-10	7.62E-11
Non carcinogenics	CTU_h	1.91E-08	1.31E-11	3.72E-15	1.82E-08	9.37E-10
Respiratory effects	Kg $PM_{2.5}$	3.32E-04	1.11E-07	1.39E-07	2.52E-04	7.97E-05
Ecotoxicity	CTU_e	3.88E-02	1.62E-04	6.35E-09	3.57E-02	2.98E-03
Fossil fuel depletion	MJ surplus	2.45E-02	1.38E-04	3.38E-06	1.71E-02	7.32E-03

Table S17. Detailed LCIA midpoint results of the separation process. The table show the contribution of each input and output on the total score of the process.

Impact category	Unit	Total	NaOH	H2SO4	Electricity	Cooling	Biogas WWT	WWT	Waste disposal
Ozone depletion	Kg CFC_{11-eq}	-1.32E-08	2.31E-10	1.20E-08	1.24E-09	5.75E-09	-3.82E-08	1.19E-11	5.78E-09
GHG emissions	Kg CO_{2-eq}	1.79E-01	6.15E-03	8.65E-02	3.29E-02	5.77E-02	-2.13E-02	1.00E-04	1.74E-02
Smog	Kg O_{3-eq}	2.29E-02	4.12E-04	1.86E-02	1.07E-03	8.79E-04	-1.19E-03	1.04E-05	3.12E-03
Acidification	Kg SO_{2-eq}	5.16E-03	6.03E-05	5.41E-03	1.13E-04	1.69E-04	-7.21E-04	9.80E-07	1.31E-04
Eutrophication	Kg N_{-eq}	3.29E-04	1.48E-05	2.32E-04	4.09E-05	2.47E-05	-9.73E-06	8.41E-06	1.73E-05
Carcinogenics	CTU_h	3.46E-09	6.22E-11	3.16E-09	1.19E-10	3.81E-10	-4.10E-10	2.78E-11	1.17E-10
Non carcinogenics	CTU_h	3.17E-08	1.73E-09	2.64E-08	1.45E-09	2.95E-09	-3.88E-09	5.78E-10	2.43E-09
Respiratory effects	Kg $PM_{2.5}$	5.85E-04	2.40E-05	4.39E-04	1.33E-04	2.03E-05	-5.71E-05	1.58E-07	2.50E-05
Ecotoxicity	CTU_e	1.36E-01	3.40E-03	1.61E-01	3.25E-03	2.51E-02	-9.12E-02	1.22E-03	3.33E-02
Fossil fuel depletion	MJ surplus	-1.13E-01	1.63E-03	1.07E-01	4.92E-03	1.38E-01	-4.16E-01	9.30E-05	5.21E-02

Table S18. Detailed LCIA midpoint results of the hydrogenation process. The table show the contribution of each input and output on the total score of the process.

Impact category	Unit	Total	Catalytic Process	Ethanol recycling	Hydrogen recycling	Adipic acid crystallization
Ozone depletion	Kg CFC_{11-eq}	2.44E-07	1.03E-07	1.35E-07	1.03E-10	5.48E-09
GHG emissions	Kg CO_{2-eq}	2.53E+00	1.12E+00	1.35E+00	1.24E-03	5.50E-02
Smog	Kg O_{3-eq}	3.83E-02	1.87E-02	1.87E-02	2.88E-05	8.37E-04
Acidification	Kg SO_{2-eq}	7.56E-03	3.58E-03	3.81E-03	3.92E-06	1.61E-04
Eutrophication	Kg N_{-eq}	7.50E-04	3.54E-04	3.71E-04	1.16E-06	2.35E-05
Carcinogenics	CTU_h	9.41E-09	2.81E-09	6.23E-09	5.47E-12	3.63E-10
Non carcinogenics	CTU_h	7.77E-08	2.62E-08	4.87E-08	5.73E-11	2.81E-09
Respiratory effects	Kg $PM_{2.5}$	9.30E-04	5.00E-04	4.07E-04	3.56E-06	1.94E-05
Ecotoxicity	CTU_e	9.85E-01	4.45E-01	5.16E-01	2.72E-04	2.39E-02
Fossil fuel depletion	Kg CFC_{11-eq}	6.51E+00	3.10E+00	3.27E+00	1.10E-03	1.31E-01

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