Multi-product biorefineries from lignocelluloses: A pathway to revitalisation of the Sugar Industry?

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Supplementary Information: 16 Tables and 1 Figure

Table S1 The main parameters implemented for the Aspen simulation of biorefinery scenarios

Parameter	*Value*	*Parameter*	*Value*
Pretreatment of Scenarios 1, 2 and 3		**Pretreatment of Scenario 4**	
Low pressure steam % wt of DM	10 %	Acid flow per biomass % wt	1.8 %
SO_2 % wt of DM	1.9 %	Cellulose→ Glucose	6.9 %
High pressure steam % wt of DM	50. %	Xylan→ Xylose	87.4 %
Cellulose→ Glucose	7.0 %	Xylan→ Furfural	5 %
Cellulose→ Acetic Acid	6.3 %	**SSF (Scenario 4)**	
Xylan→ Xylose	80.1 %	Cellulose→ Glucose	95.0 %
Xylan→ Furfural	3.1 %	Xylan→ Xylose	95.0 %
SSCF (Scenario 1)		Glucose → Butanol	55.7 %
Cellulose→ Glucose	74.5%	Glucose → Ethanol	6.6 %
Glucose → Ethanol	90.5 %	Glucose → Acetone	31.1 %
Xylose → Ethanol	76.6 %	Xylose → Butanol	20.1 %
Ethanol concentration % wt	5.5 %	Xylose → Ethanol	4.2 %
Xylose fermentation Scenario 2		Xylose → Acetone	18.5 %
Xylose → Lactic Acid	95.0 %	**Gasification (Scenarios 5 and 6)**	
Xylose fermentation Scenario 3		Feedstock split % wt of DM	42 %
Xylose → Furfural	83.0 %	Steam for gasification % wt of DM	100 %
In common units			
Boiler unit		**Steam and power unit**	
Deaerator pressure	3.3 atm	Number of extractions	3
Deaerator temperature	108 °C	Turbine isotropic efficiency	85 %
Boiler feed water pressure	62.2 atm	Mechanical efficiency	96 %
Boiler feed water temperature	176 °C	Sugar mill's steam extraction	27.6 atm
HHP steam pressure	62.2 atm	1st extraction pressure	13 atm
HHP steam temperature	452 °C	2nd extraction pressure	9.5 atm
Averaged burner temperature	870 °C	Condensate turbine pressure	0.1 atm
Combustion conversion	98 %	**Wastewater treatment unit**	
Inlet economizer temperature	278 °C	Wastewater temperature	35 °C
Air preheat temperature	185 °C	Chemical oxygen demand (COD)	16 g/L
Stack temperature	149 °C	Biological oxygen demand per COD	70 %
Boiler heat loss (total)	5%	Organic component → $3CH4 + CO_2$	90 %
Evaporation unit		Methane to removed COD @ 25°C	0.23 kg/kg
First effect pressure	0.385 atm	Nutrient (per COD)	37 g/kg
LPS % of liquid inlet	5 %	COD of treated water	0.1 g/L
Second effect pressure	0.26 atm		
Third effect pressure	0.21 atm		
Forth effect pressure	0.16 atm		

Table S2 Utilities condition of the developed biorefinery scenarios

	Supplied		Return	
	Temperature (°C)	Pressure (atm)	Temperature (°C)	Pressure (atm)
Chilled water	4	2	15	1
Cooling water	28	2	37	1
Cooling air	30	1	35	1
High pressure steam (HPS)	266	13	192	12
Low pressure steam (LPS)	233	9.5	170	8
Sugar mill steam demand	338	27.6	122	2.2

Table S3 The specific energy consumption of the studied biorefinery scenarios (data of Figure 4)

	Cooling (kW/t*)	Heating (kW/t*)	Power (kW/t*)
Scenario 1: Ethanol	1198.8	1634.9	48.0
Scenario 2: Ethanol, LA	1166.5	1707.8	51.3
Scenario 3: Ethanol, Furfural	1599.9	2041.1	71.7
Scenario 4: Butanol	1873.7	822.3	580.6
Scenario 5: Methanol	620.6	61.8	335.4
Scenario 6: FTS	744.6	51.9	300.7

*****: Specific energy consumption is defined as: kW of consumed energy per tonne feedstock to biorefinery (kw/t)

Table S4 The detailed sales of the studied scenarios (data of Figure 6)

	Sales (M $)											
	Total	Electricity	Ethanol	lactic acid	furfural	butanol	Formic acid	Acetic Acid	HMF	Acetone	methanol	FT syncrude
Scenario 1	58.58	3.9	54.7	0.0	0.0	-	-	-	-	-	-	-
Scenario 2	99.53	2.2	37.2	60.2	0.0	-	-	-	-	-	-	-
Scenario 3	54.03	4.1	28.5	0.0	16.4	-	0.8	3.5	0.8	-	-	-
Scenario 4	40.17	2.4	1.9	0.0	0.0	30.4	-	-	-	5.6	-	-
Scenario 5	56.5	0.3	0.0	0.0	0.0	-	-	-	-	-	56.2	-
Scenario 6	12.64	1.1	0.0	0.0	0.0	-	-	-	-	-	-	11.5

Table S5 Inventory for Sugarcane Cultivation*

Sugar cane agriculture	**Value**	**unit**
Cultivation area	400000	ha
Average cane harvest	60	t/ha
Irrigation water requirements	8000	m^3/ha
Electricity consumption for irrigation	108	kWh/ha
N_2O emissions from soil	1.5(1.25% of N input)	kg
NO_x emissions from soil	0.6(0.5% of N input)	kg
Fertilizer application rate/ha		
Urea, N	120	kg
Diammonium phosphate (DAP), P_2O_5	30	kg
Potassium oxide, KCl	125	kg
Herbicides use	1614(26.9g/ton sugar cane)	g
Herbicides loss in water bodies	3.228(0.2%)	g
Nitrogen loss in water bodies	161.4(10%)	g
Phosphorus loss in surface runoff/ha	1	kg
Pesticide use	132.6	g
Cane transportation		
Transportation, average distance, by:		
road(94% of cane)	25	km
rail(6% of cane)	50	km
Diesel consumption:		
Truck	1.08	MJ/tkm
rail	0.68	MJ/tkm
Fertilizers and herbicides transport distance	60	km

***Mashoko, L., Mbohwa, C., Thomas, V.M., 2010. LCA of the South African Sugar Industry. J. Environ. Plan. Manag. 53, 793–807**

Table S6 Inventory for Sugarcane processing in the sugar mill*

Sugar processing	
Sugarcane	6.0t
Bagasse produced	27.8% of cane
Molasses produced	4.1% of cane
Filter cake produced	6.8% of cane
Steam consumed/t of cane	520kg
Electricity consumption/t of cane	35kWh
Electricity generation/t of cane	150kWh
Coal consumption/t of cane	8.4kg
Water used for cane processing/t cane	0.6m3
Pollutant loadings of COD/t of cane	3320
Pollutant loadings of BOD5/t of cane	1590

*Mashoko, L., Mbohwa, C., Thomas, V.M., 2010. LCA of the South African Sugar Industry. J. Environ. Plan. Manag. 53, 793–807

Table S7 Inventory for the investigated biorefinery scenarios (per 65 ton/hour biomass processed)

Inputs (Feedstock and Chemicals)	EtOH	EtOH & Lactic acid	EtOH & Furfural	Butanol	Methanol	FT syncrude
Bagasse and brown leaves (kg)	6.50E+04	6.50E+04	6.50E+04	6.50E+04	6.50E+04	6.50E+04
Sulphure	2.77E+02	2.10E+02	2.43E+02	-	-	-
Sulphuric acid (93%) (kg)	4.00E-01	3.68E-01	3.07E-01	2.55E+02	-	-
Ammonia (kg)	3.00E+01	3.31E+01	1.37E+01	8.22E+02	-	-
Diammonium phosphate (kg)	4.40E+01	9.43E+01	3.75E+01	-	-	-
Triethylamine (TEA) (kg)	-	1.09E+02	-	-	-	-
$MgSO_4$	-	5.00E+01	-	-	-	-
$Mg(OH)_2$	-	5.50E+00	-	-	-	-
Glucose (kg)	7.54E+02	6.96E+02	6.38E+02	-	-	-
Boiler & cooling tower Chemicals (kg)	3.00E+02	3.00E+02	3.00E+02	3.00E+02	2.50E+02	2.50E+02
NaoCl (kg)	5.70E+00	5.06E+00	6.40E+00	3.60E+00	-	-
Tetrahydrofuran (THF) (kg)	-	-	6.43E+02	-	-	-
NaCl (kg)	-	-	2.00E+03	-	-	-
HCl (kg)	-	-	1.05E+03	-	-	-
Outputs						
Ethanol production (kg)	1.10E+04	6.73E+03	5.66E+03	3.53E+02	-	-
Lactic acid production (kg)	-	4.65E+03	-	-	-	-
Furfural Production (kg)	-	-	2.07E+03	-	-	-
Acetic acid (kg)	-	-	1.25E+03	-	-	-
Formic acid (kg)	-	-	2.28E+02	-	-	-
Butanol production (kg)	-	-	-	4.61E+03	-	-
Aceton (kg)	-	-	-	1.48E+03	-	-
Methanol production (kg)	-	-	-	-	1.28E+04	-
FT syncrude production (kg)	-	-	-	-	-	5.81E+03
Exported electricity (MW)	7.10E+00	5.60E+00	7.50E+00	4.30E+00	5.00E-01	1.80E+00
Emissions and waste disposal						
EtOH (kg)	9.82E-01	1.82E+01	4.24E+00	6.01E+00	-	-
CO_2 (kg)	8.99E+04	9.42E+04	8.89E+04	9.63E+04	5.87E+04	5.79E+04
SO_2 (kg)	1.63E+01	1.85E+01	7.60E+00	8.56E+00	-	-
Acetic Acid (kg)	6.43E+00	7.46E+00	1.69E+00	6.60E-01	-	-
Furfural (kg)	2.02E+00	1.96E+00	4.48E-01	2.77E-01	-	-
CH_4 (kg)	2.28E+00	2.28E+00	1.58E+00	-	-	6.42E+01
NO_2 (kg)	4.60E-02	4.60E-02	4.60E-02	4.60E-02	3.75E+00	3.08E+00
CO	3.00E-03	3.00E-03	3.00E-03	4.00E-03	7.76E+01	7.76E+01
Acetone (kg)	-	-	-	1.73E+02	-	-
NO (kg)	-	-	-	-	2.01E+02	1.66E+02
C_4H_{10} (kg)	-	-	-	-	-	5.47E+00
Landfill disposal of ash (kg)	3.25E+03	3.04E+03	3.10E+03	2.28E+03	7.88E+02	7.88E+02

Table S8 LCIA profiles of bioethanol production (unit: 1ton bioethanol; method: CML-IA baseline V3.02)

Impact category	Unit	Total	Pre-treatment	Enzyme production	SSCH	EtOH purification	Evaporation	Combustion	Waste water treatment	Biomass production	AD
Abiotic depletion	kg Sb eq	4.51E-04	1.90E-06	2.26E-05	6.10E-06	0.00E+00	0.00E+00	2.62E-05	2.20E-06	3.90E-04	2.14E-06
Abiotic depletion(fossil fuel)	MJ	1.93E+03	3.90E+02	9.87E+01	6.50E+01	0.00E+00	0.00E+00	3.76E+02	6.02E+00	9.95E+02	3.27E+00
GWP_{100}	kg CO_2 eq	4.57E+03	3.61E+00	9.10E+01	3.84E+00	5.21E+02	0.00E+00	3.87E+03	3.37E-01	8.24E+01	2.71E-01
ODP	kg CFC-11 eq	4.44E-05	4.11E-06	6.27E-06	7.79E-07	0.00E+00	0.00E+00	3.16E-06	6.87E-08	2.99E-05	1.27E-07
Human toxicity	kg 1,4-DB eq	1.19E+03	9.85E-01	2.06E+01	1.89E+00	1.84E-02	0.00E+00	1.03E+03	2.61E-01	1.39E+02	1.77E-01
Fresh water eco-toxicity	kg 1,4-DB eq	3.13E+02	4.26E-01	4.88E+00	3.51E-01	0.00E+00	0.00E+00	2.85E+02	7.27E-02	2.22E+01	1.26E-01
Marine aquatic eco-toxicity	kg 1,4-DB eq	3.86E+05	1.50E+03	4.52E+04	1.24E+03	0.00E+00	0.00E+00	2.59E+05	3.22E+02	7.80E+04	3.90E+02
Terrestrial eco-toxicity	kg 1,4-DB eq	9.75E-01	6.04E-03	1.29E-01	6.11E-03	0.00E+00	0.00E+00	6.66E-01	9.89E-04	1.66E-01	1.24E-03
POCP	kg C_2H_4 eq	1.57E-01	2.28E-03	2.09E-02	1.31E-03	1.64E-02	2.12E-02	2.34E-02	3.16E-02	3.95E-02	7.88E-05
Acidification	kg SO_2 eq	2.27E+00	3.86E-02	5.35E-01	2.77E-02	2.30E-01	0.00E+00	2.02E-01	6.38E-01	5.96E-01	1.88E-03
Eutrophication	kg PO_4^{3-} eq	2.26E+00	5.17E-03	4.59E-01	2.54E-03	1.36E-01	0.00E+00	1.37E+00	5.78E-04	2.77E-01	6.56E-04

Table S9 LCIA profiles of bioethanol and lactic acid production (unit: 1ton Lactic acid; method: CML-IA baseline V3.02)

Impact category	Unit	Total	Pre-treatment	Enzyme production	SSCH	EtOH purification	Evaporation	Combustion	Waste water treatment	Biomass production	AD	Lactic Acid production
Abiotic depletion	kg Sb eq	8.24E-04	2.32E-06	3.68E-05	8.91E-06	0.00E+00	0.00E+00	3.86E-05	3.47E-06	6.15E-04	3.00E-06	1.16E-04
Abiotic depletion(fossil fuel)	MJ	3.49E+03	4.66E+02	1.66E+02	9.49E+01	0.00E+00	0.00E+00	5.54E+02	9.48E+00	1.57E+03	4.57E+00	6.30E+02
GWP_{100}	kg CO_2 eq	7.41E+03	4.31E+00	1.34E+02	5.61E+00	5.67E+02	0.00E+00	6.54E+03	5.32E-01	1.30E+02	3.80E-01	2.39E+01
ODP	kg CFC-11 eq	6.99E-05	4.91E-06	9.38E-06	1.14E-06	0.00E+00	0.00E+00	4.65E-06	1.08E-07	4.71E-05	1.78E-07	2.40E-06
Human toxicity	kg 1,4-DB eq	1.79E+03	1.18E+00	3.07E+01	2.77E+00	1.09E-02	0.00E+00	1.52E+03	4.41E-01	2.19E+02	2.47E-01	1.83E+01
Fresh water eco-toxicity	kg 1,4-DB eq	4.70E+02	5.10E-01	7.26E+00	5.12E-01	0.00E+00	0.00E+00	4.20E+02	1.15E-01	3.51E+01	1.76E-01	5.75E+00
Marine aquatic eco-toxicity	kg 1,4-DB eq	5.97E+05	1.79E+03	6.63E+04	1.82E+03	0.00E+00	0.00E+00	3.82E+05	5.07E+02	1.23E+05	5.46E+02	2.11E+04
Terrestrial eco-toxicity	kg 1,4-DB eq	1.50E+00	7.22E-03	1.90E-01	8.92E-03	0.00E+00	0.00E+00	9.81E-01	1.56E-03	2.62E-01	1.73E-03	4.94E-02
POCP	kg C_2H_4 eq	7.86E-01	2.73E-03	3.08E-02	1.92E-03	1.15E-02	3.15E-01	5.30E-02	2.98E-01	6.23E-02	1.10E-04	1.11E-02
Acidification	kg SO_2 eq	3.87E+00	4.62E-02	7.87E-01	4.04E-02	1.37E-01	0.00E+00	3.78E-01	1.37E+00	9.40E-01	2.63E-03	1.64E-01
Eutrophication	kg PO_4^{3-} eq	3.29E+00	6.18E-03	6.68E-01	3.72E-03	1.08E-01	0.00E+00	2.03E+00	9.11E-04	4.37E-01	9.19E-04	4.10E-02

Table S10 LCIA profiles of bioethanol and furfural production (unit: 1ton Furfural; method: CML-IA baseline V3.02)

Impact category	Unit	Total	Pre-treatment	Enzyme production	SSCH	EtOH purification	Evaporation	Combustion	Waste water treatment	Biomass production	AD	Furfural production
Abiotic depletion	kg Sb eq	2.98E-03	2.74E-06	2.71E-05	7.54E-06	0.00E+00	0.00E+00	4.16E-05	3.66E-06	6.50E-04	4.01E-06	2.24E-03
Abiotic depletion(fossil fuel)	MJ	9.41E+03	5.70E+02	8.93E+01	8.03E+01	0.00E+00	0.00E+00	5.97E+02	1.00E+01	1.66E+03	6.12E+00	6.40E+03
GWP_{100}	kg CO_2 eq	7.91E+03	5.28E+00	1.25E+02	4.74E+00	4.72E+02	0.00E+00	6.76E+03	5.63E-01	1.37E+02	5.08E-01	4.00E+02
ODP	kg CFC-11 eq	1.40E-04	6.01E-06	8.24E-06	9.62E-07	0.00E+00	0.00E+00	5.02E-06	1.14E-07	4.98E-05	2.37E-07	6.99E-05
Human toxicity	kg 1,4-DB eq	2.11E+03	1.44E+00	2.76E+01	2.34E+00	8.47E-03	0.00E+00	1.64E+03	3.97E-01	2.31E+02	3.31E-01	2.11E+02
Fresh water eco-toxicity	kg 1,4-DB eq	6.48E+02	6.22E-01	6.60E+00	4.33E-01	0.00E+00	0.00E+00	4.53E+02	1.21E-01	3.71E+01	2.36E-01	1.50E+02
Marine aquatic eco-toxicity	kg 1,4-DB eq	1.07E+06	2.19E+03	6.27E+04	1.54E+03	0.00E+00	0.00E+00	4.12E+05	5.36E+02	1.30E+05	7.31E+02	4.58E+05
Terrestrial eco-toxicity	kg 1,4-DB eq	2.77E+00	8.83E-03	1.77E-01	7.54E-03	0.00E+00	0.00E+00	1.06E+00	1.65E-03	2.77E-01	2.32E-03	1.24E+00
POCP	kg C_2H_4 eq	4.35E-01	3.33E-03	2.84E-02	1.62E-03	7.11E-03	1.03E-01	1.94E-02	5.94E-02	6.59E-02	1.48E-04	1.46E-01
Acidification	kg SO_2 eq	5.49E+00	5.65E-02	7.32E-01	3.42E-02	1.06E-01	0.00E+00	3.12E-01	5.83E-01	9.94E-01	3.52E-03	2.67E+00
Eutrophication	kg PO_4^{3-} eq	4.26E+00	7.56E-03	6.44E-01	3.14E-03	5.73E-02	0.00E+00	2.18E+00	9.63E-04	4.62E-01	1.23E-03	8.99E-01

Table S11 LCIA profiles of butanol production (unit: 1ton butanol; method: CML-IA baseline V3.02)

Impact category	Unit	Total	Pre-treatment	SSF	Combustion	Seed generation	Biomass production
Abiotic depletion	kg Sb eq	1.16E-03	2.34E-04	2.66E-04	2.95E-05	9.07E-07	6.26E-04
Abiotic depletion(fossil fuel)	MJ	5.33E+03	4.68E+02	2.83E+03	4.23E+02	9.66E+00	1.60E+03
GWP_{100}	kg CO_2 eq	7.83E+03	2.28E+01	1.04E+03	6.63E+03	5.71E-01	1.32E+02
ODP	kg CFC-11 eq	9.09E-05	5.39E-06	3.39E-05	3.55E-06	1.16E-07	4.80E-05
Human toxicity	kg 1,4-DB eq	1.48E+03	1.60E+01	8.24E+01	1.16E+03	2.81E-01	2.23E+02
Fresh water eco-toxicity	kg 1,4-DB eq	3.78E+02	5.80E+00	1.53E+01	3.21E+02	5.21E-02	3.57E+01
Marine aquatic eco-toxicity	kg 1,4-DB eq	4.88E+05	1.66E+04	5.42E+04	2.92E+05	1.85E+02	1.25E+05
Terrestrial eco-toxicity	kg 1,4-DB eq	1.32E+00	4.13E-02	2.66E-01	7.49E-01	9.08E-04	2.66E-01
POCP	kg C_2H_4 eq	1.67E+00	1.32E-02	1.55E+00	4.01E-02	1.95E-04	6.35E-02
Acidification	kg SO_2 eq	3.44E+00	3.02E-01	1.20E+00	9.76E-01	4.11E-03	9.57E-01
Eutrophication	kg PO_4^{3-} eq	2.13E+00	2.93E-02	1.11E-01	1.55E+00	3.78E-04	4.45E-01

Table S12 LCIA profiles of methanol production (unit: 1ton Methanol; method: CML-IA baseline V3.02)

Impact category	Unit	Total	Gasification & Conditioning	Combustion	Biomass production
Abiotic depletion	kg Sb eq	3.89E-04	0.00E+00	7.81E-06	3.82E-04
Abiotic depletion(fossil fuel)	MJ	1.09E+03	0.00E+00	1.12E+02	9.76E+02
GWP_{100}	kg CO_2 eq	2.87E+03	5.33E+02	2.25E+03	8.07E+01
ODP	kg CFC-11 eq	3.02E-05	0.00E+00	9.41E-07	2.93E-05
Human toxicity	kg 1,4-DB eq	4.54E+02	0.00E+00	3.19E+02	1.36E+02
Fresh water eco-toxicity	kg 1,4-DB eq	1.07E+02	0.00E+00	8.50E+01	2.18E+01
Marine aquatic eco-toxicity	kg 1,4-DB eq	1.54E+05	0.00E+00	7.73E+04	7.64E+04
Terrestrial eco-toxicity	kg 1,4-DB eq	3.61E-01	0.00E+00	1.99E-01	1.63E-01
POCP	kg C_2H_4 eq	1.44E-01	9.84E-02	7.28E-03	3.87E-02
Acidification	kg SO_2 eq	5.43E+00	0.00E+00	4.85E+00	5.84E-01
Eutrophication	kg PO_4^{3-} eq	1.93E+00	0.00E+00	1.66E+00	2.71E-01

Table S13 LCIA profiles of FT syncrude production (unit: 1ton FT syncrude; method: CML-IA baseline V3.02)

Impact category	Unit	Total	Gasification & Conditioning	Combustion	FT synthesis	Biomass production
Abiotic depletion	kg Sb eq	4.49E-04	0.00E+00	9.00E-06	0.00E+00	4.40E-04
Abiotic depletion(fossil fuel)	MJ	1.25E+03	0.00E+00	1.29E+02	0.00E+00	1.12E+03
GWP_{100}	kg CO_2 eq	3.35E+03	6.15E+02	2.55E+03	9.56E+01	9.30E+01
ODP	kg CFC-11 eq	3.48E-05	0.00E+00	1.09E-06	0.00E+00	3.37E-05
Human toxicity	kg 1,4-DB eq	5.21E+02	0.00E+00	3.65E+02	0.00E+00	1.57E+02
Fresh water eco-toxicity	kg 1,4-DB eq	1.23E+02	0.00E+00	9.80E+01	0.00E+00	2.51E+01
Marine aquatic eco-toxicity	kg 1,4-DB eq	1.77E+05	0.00E+00	8.90E+04	0.00E+00	8.81E+04
Terrestrial eco-toxicity	kg 1,4-DB eq	4.16E-01	0.00E+00	2.29E-01	0.00E+00	1.87E-01
POCP	kg C_2H_4 eq	5.58E-01	1.13E-01	7.32E-03	3.93E-01	4.46E-02
Acidification	kg SO_2 eq	5.31E+00	0.00E+00	4.64E+00	0.00E+00	6.73E-01
Eutrophication	kg PO_4^{3-} eq	1.99E+00	0.00E+00	1.66E+00	1.77E-02	3.13E-01

Table S14 LCIA profiles for comparison of biorefinery scenarios (method: CML-IA baseline V3.02)

Impact category	Unit	EtOH	EtOH & Lactic acid	EtOH & Furfural	Butanol	Methanol	FT syntcrude
Abiotic depletion	kg Sb eq	8.82E-03	1.03E-02	3.65E-02	7.48E-03	7.86E-04	7.86E-04
Abiotic depletion(fossil fuel)	MJ	3.88E+04	4.47E+04	1.16E+05	5.19E+04	6.02E+03	6.02E+03
GWP_{100}	kg CO_2 eq	9.49E+04	9.76E+04	9.85E+04	9.99E+04	5.94E+04	6.03E+04
ODP	kg CFC-11 eq	8.81E-04	8.79E-04	1.71E-03	5.94E-04	5.76E-05	5.76E-05
Human toxicity	kg 1,4-DB eq	2.46E+04	2.34E+04	2.61E+04	1.64E+04	6.89E+03	6.85E+03
Fresh water eco-toxicity	kg 1,4-DB eq	6.48E+03	6.16E+03	8.05E+03	4.48E+03	1.86E+03	1.86E+03
Marine aquatic eco-toxicity	kg 1,4-DB eq	7.91E+06	7.76E+06	1.32E+07	4.86E+06	1.81E+06	1.81E+06
Terrestrial eco-toxicity	kg 1,4-DB eq	2.00E+01	1.96E+01	3.44E+01	1.42E+01	4.74E+00	4.74E+00
POCP	kg C_2H_4 eq	3.20E+00	1.03E+01	5.37E+00	2.08E+01	2.30E+00	9.53E+00
Acidification	kg SO_2 eq	4.63E+01	5.01E+01	6.76E+01	3.36E+01	1.04E+02	8.68E+01
Eutrophication	kg PO_4^{3-} eq	4.65E+01	4.30E+01	5.27E+01	2.23E+01	3.56E+01	3.14E+01

Table S15 LCIA profiles for comparison of different scenarios for production of 1 tonne bioethanol (method: CML-IA baseline V3.02)

Impact category	Unit	EtOH	EtOH & Lactic acid	EtOH & Furfural
Abiotic depletion	kg Sb eq	7.98E-04	6.76E-04	3.50E-03
Abiotic depletion(fossil fuel)	MJ	3.43E+03	2.87E+03	1.11E+04
GWP_{100}	kg CO_2 eq	8.09E+03	6.08E+03	9.29E+03
ODP	kg CFC-11 eq	7.86E-05	5.74E-05	1.65E-04
Human toxicity	kg 1,4-DB eq	2.11E+03	1.47E+03	2.48E+03
Fresh water eco-toxicity	kg 1,4-DB eq	5.55E+02	3.85E+02	7.62E+02
Marine aquatic eco-toxicity	kg 1,4-DB eq	6.83E+05	4.90E+05	1.25E+06
Terrestrial eco-toxicity	kg 1,4-DB eq	1.73E+00	1.23E+00	3.26E+00
POCP	kg C_2H_4 eq	2.77E-01	6.45E-01	5.11E-01
Acidification	kg SO_2 eq	4.02E+00	3.17E+00	6.45E+00
Eutrophication	kg PO_4^{3-} eq	3.99E+00	2.70E+00	5.00E+00

Table S16 LCIA profiles for comparison of biorefinery scenarios (method: EI 99H)

Impact category	Unit	EtOH	EtOH & Lactic acid	EtOH & Furfural	Butanol	Methanol	FT syntcrude
Carcinogens	DALY	7.08E-03	6.77E-03	8.60E-03	5.11E-03	2.04E-03	2.04E-03
Resp. organics	DALY	5.28E-06	2.01E-05	1.17E-05	4.40E-05	4.26E-07	5.39E-06
Resp. inorganics	DALY	4.21E-03	4.52E-03	7.55E-03	3.27E-03	1.86E-02	1.55E-02
Climate change	DALY	1.99E-02	2.05E-02	2.07E-02	2.10E-02	1.25E-02	1.27E-02
Radiation	DALY	8.04E-06	8.23E-06	2.48E-05	6.70E-06	9.49E-07	9.49E-07
Ozone layer	DALY	9.76E-07	9.75E-07	2.09E-06	6.21E-07	5.99E-08	5.99E-08
Ecotoxicity	PAF*m^2yr	5.56E+03	5.37E+03	7.50E+03	5.26E+03	1.58E+03	1.58E+03
Acidification/Eutrophication	PDF*m^2yr	1.28E+02	1.30E+02	2.00E+02	6.31E+01	1.18E+03	9.78E+02
Land use	PDF*m^2yr	8.08E+01	8.77E+01	1.26E+01	2.96E+01	1.19E+01	1.19E+01
Minerals	MJ surplus	8.67E+01	9.81E+01	3.81E+02	7.21E+01	1.20E+01	1.20E+01
Fossil fuels	MJ surplus	4.23E+03	4.93E+03	1.17E+04	6.58E+03	6.51E+02	6.51E+02

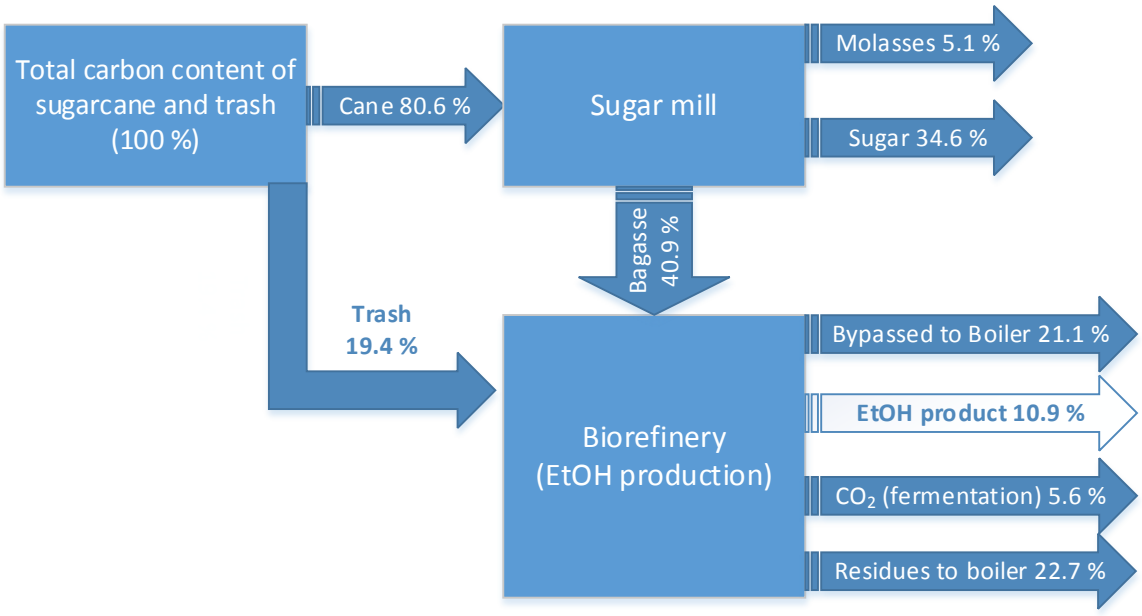

Figure S1 A schematic diagram of carbon flows through a biorefinery scenario (from sugarcane to final products).