Supplementary Material

1. Simulation of sugarcane combustion

1.1. General scheme

The heat and power generation from the combustion of sugarcane in a Mexican mill was simulated using Aspen Plus v9.0 using data from literature and primary sources. Figure S1 shows a schematic diagram of this system. First, the biomass is burnt in a furnace, the resulting ashes and combustion gases are separated. The amount of air was estimated considering the required oxygen to undertake complete combustion (according to stoichiometry) and a typical excess of 50%. The hot combustion gases are then cooled down in a heat exchanger to generate high-pressure steam, subsequently generating heat and power. The following sections explain in more detail the assumptions of the simulation.

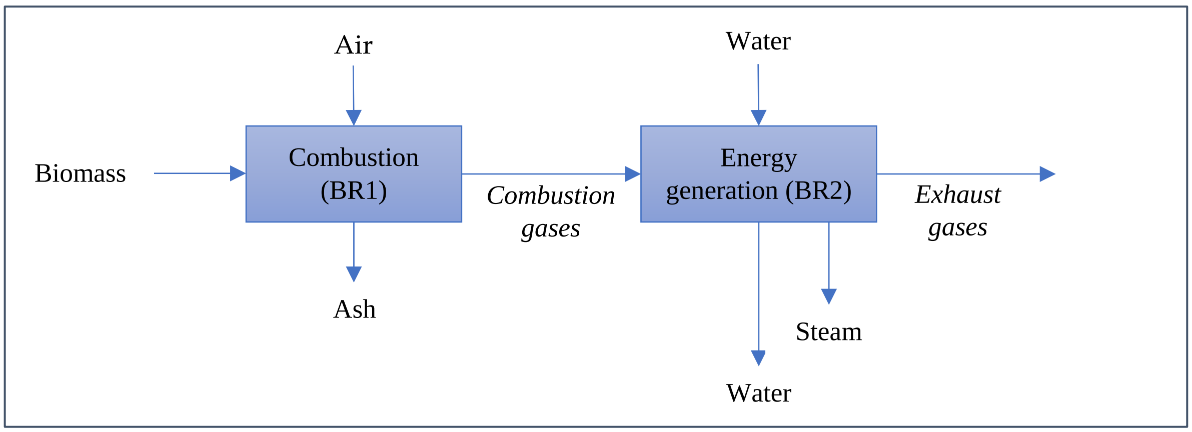

Figure S1. Schematic diagram of the heat and power generation from biomass.

1.2. Composition of air and biomass

1.2.1. Chemical composition of the air

The chemical composition of the air was simulated considering the weather conditions of Veracruz, Mexico, and Lenntech´s relative humidity calculator [1,2]. Table S1 shows the resulting chemical composition of the air.

Table S1. Chemical composition of the air.

Compound	Unit	Value
Water content in the air	g/kg	14.10
N_2	mol/mol	78.084000
O_2	mol/mol	20.946000
H_2	mol/mol	0.000055
CO_2	mol/mol	0.035000
CO	mol/mol	0.000010
N_2O	mol/mol	0.000030
NO_2	mol/mol	0.000002
Argon	mol/mol	0.934000
CH_4	mol/mol	0.000179

Source: Own elaboration based on the weather conditions of Veracruz, Mexico, and Lenntech´s relative humidity calculator **[1,2]**.

1.2.2. Chemical composition of the biomass

Sugarcane bagasse was modeled as a non-conventional solid whose chemical composition (provided by the sugarcane facility) is summarized in Table S2.

Table S2. Chemical composition of the biomass.

Parameter	Unit	Value
Calorific value	MJ/kg	15.1
Ultanal analysis		
Carbon	w/w	46.2%
Hydrogen	w/w	5.6%
Oxygen	w/w	45.6%
Nitrogen	w/w	0.2%
Chlorine	w/w	0.0%
Sulfur	w/w	0.2%
Ash	w/w	2.2%
Proximal analysis		
Moisture	w/w	49.3%
Fixed carbon	w/w	14.0%
Volatile matter	w/w	80.4%

Source: Sugarcane facility. Questionaries.

1.3. Simulation

1.3.1. General simulation scheme

Figure S2 shows the general scheme of the simulation of sugarcane combustion. The activities involved in this process were gathered in a set of hierarchies according to the schematic diagram in Figure S2. Thus, blocks B1 and B2 refer to the combustion and energy processes, respectively. The Peng-Robinson equation of state with Boston-Mathias modifications (PR-BM) thermodynamic model was used to perform the simulation according to the metrics established by guidelines of the Aspen Plus software on handling solids [3]. A flow of 375,874 t of biomass (wet basis) per year (4237 hours per year) was used as a computation base of the simulation to model the real-life conditions of the combustion of sugarcane bagasse in a Mexican mill. Both the reference and the alternative systems have the same general simulation scheme.

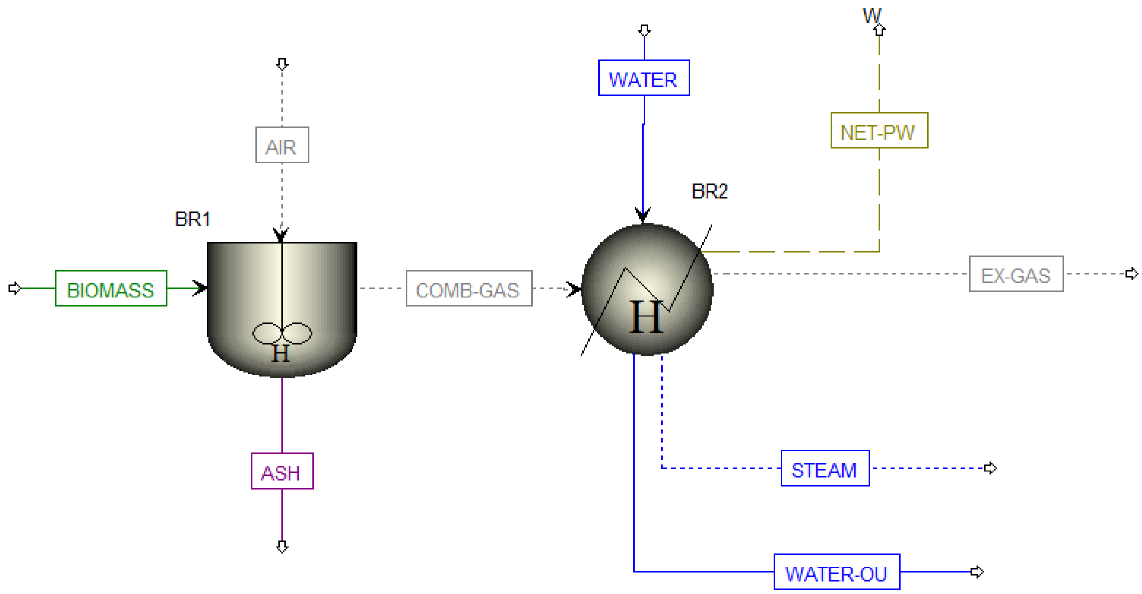

Figure S2. General scheme of the simulation of biomass combustion.

Source: Own elaboration.

Table S3 summarizes the mass balance of the reference and alternative scenarios. In both cases, the sugarcane mill requires 95 MW heat for internal purposes, which are fulfilled by the combustion of the sugarcane bagasse. However, in the reference scenario, the mill generates 5 MWe, which implies an electrical efficiency of 2.6% or the generation of 0.11 kWhe per kg of dry biomass. In the alternate scenario, on the other hand, the mill generates 12 MWe power, which implies an electrical efficiency of 6.3% or the generation of 0.26 kWhe per kg of dry biomass. The following sections explain in detail each of the hierarchies of the general scheme of the simulation (Figure S2).

Simulation of the hierarchy BR1

Figure S3 shows the simulation scheme of the hierarchy BR1, which models the combustion of the sugarcane bagasse depicted in Figure S1. Table S4 shows the input data of the blocks simulated in this hierarchy and their results. These conditions are the same for both the reference and alternative scenarios.

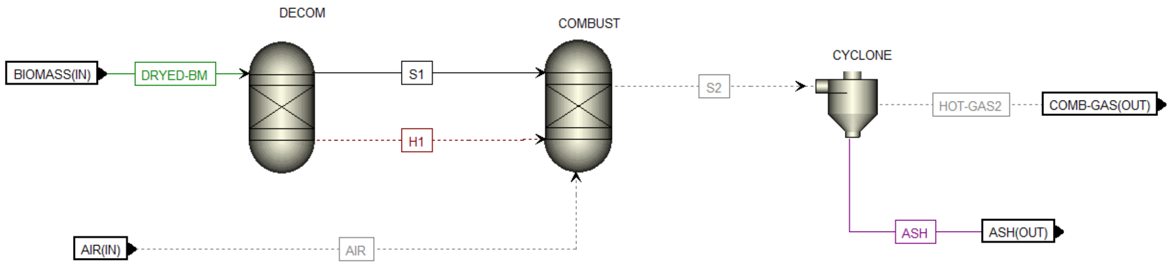

Figure S3. Scheme of the hierarchy BR1, the combustion stage**.**

Source: Own elaboration.

Table S3. Results of the main streams of the simulation.

Parameter	Unit	Input streams			Output streams – Reference scenario[a]				Output streams – Alternative scenario			
		Biomass	Air	Water	Ash	Water-out	Steam	EX-Gas	Ash	Water-Out	Steam	EX-Gas
Generalities												
Temperature	ºC	26	26	32	936	43	43	280	936	—	101	170
Pressure	atm	1	1	1	1	0.084	0.084	1	1	—	1	1
Flow (mass)	kg/h	88,712	360,742	139,426	1,010	2,647	21,880	448,444	1,010	0	139,426	448,444
Flows												
Sugarcane bagasse	kg/h	88,712	0	0	0	0	0	0	0	0	0	0
Ash	kg/h	0	0	0	1,010	0	0	0	1,010	0	0	0
N_2	kg/h	0	268,599	0	0	0	0	268,660	0	0	0	268,660
O_2	kg/h	0	82,286	0	0	0	0	27,366	0	0	0	27,366
H_2O	kg/h	0	5,086	139,426	0	2,647	21,880	71,228	0	0	139,426	71,228
H_2	kg/h	0	<0.01	0	0	0	0	<0.001	0	0	0	<0.001
CO_2	kg/h	0	189	0	0	0	0	76,427	0	0	0	76,427
CO	kg/h	0	<0.03	0	0	0	0	<0.005	0	0	0	<0.005
N_2O	kg/h	0	0.16	0	0	0	0	0	0	0	0	0
NO_2	kg/h	0	0	0	0	0	0	1	0	0	0	1
NO	kg/h	0	0	0	0	0	0	49	0	0	0	49
SO_2	kg/h	0	0	0	0	0	0	125	0	0	0	125
SO_3	kg/h	0	0	0	0	0	0	8	0	0	0	8
Ar	kg/h	0	4,581	0	0	0	0	4,581	0	0	0	4,581

[a] In this scenario there is another stream of steam used to provide the required heat for internal purposes (95 MW heat) with a flow of 114,899 kg/h at 312 °C and 15 atm.

Source: Own elaboration.

Table S4. Input data and results of the blocks in the hierarchy B1.

Equipment	Simulation block	Input data	Results
DECOM	RYield	Temperature: 26 °C Pressure: 1 atm	Heat duty: 99.5 MW
COMBUST	RGibss	Calculate option: Calculate phase equilibrium and chemical equilibrium Pressure: 1 atm	Outlet temperature: 936 °C Pressure: 1 atm Heat duty: -99.5 kW

Source: Own elaboration.

Table S5. shows the results of the main streams of the hierarchy BR1. These results are the same for both the reference and alternative scenarios.

Table S5. Results of the main streams of the hierarchy BR1.

Parameter	Unit	Input streams		Output streams	
		BIOMASS	AIR	ASH	EX-GAS
Generalities					
Temperature	ºC	26	26	936	936
Pressure	atm	1	1	1	1
Flow (mass)	kg/h	88,712	360,742	1,010	448,444
Flows					
Sugarcane bagasse	kg/h	88,712	0	0	0
Ash	kg/h	0	0	1,010	0
N_2	kg/h	0	268,599	0	268,660
O_2	kg/h	0	82,286	0	27,366
H_2O	kg/h	0	5,086	0	71,228
H_2	kg/h	0	<0.01	0	<0.001
CO_2	kg/h	0	189	0	76,427
CO	kg/h	0	<0.03	0	<0.005
N_2O	kg/h	0	0.16	0	0
NO_2	kg/h	0	0	0	1
NO	kg/h	0	0	0	49
SO_2	kg/h	0	0	0	125
SO_3	kg/h	0	0	0	8
Ar	kg/h	0	4,581	0	4,581

Source: Own elaboration.

Simulation of the hierarchy BR2

Figure S4 shows the simulation scheme of the hierarchy BR2 under the reference scenario, where a flow of 114,899 kg/h of steam (at 312 °C and 15 atm) is taken to cover the internal heat requirements of the sugarcane mill. In contrast, the remaining steam (24,527 kg/h) is used to generate electricity. Unlike other simulation blocks, the thermodynamic model of the heat exchanger was changed to ASME 1967 steam tables correlation (STEAM-TA) for its cold side.

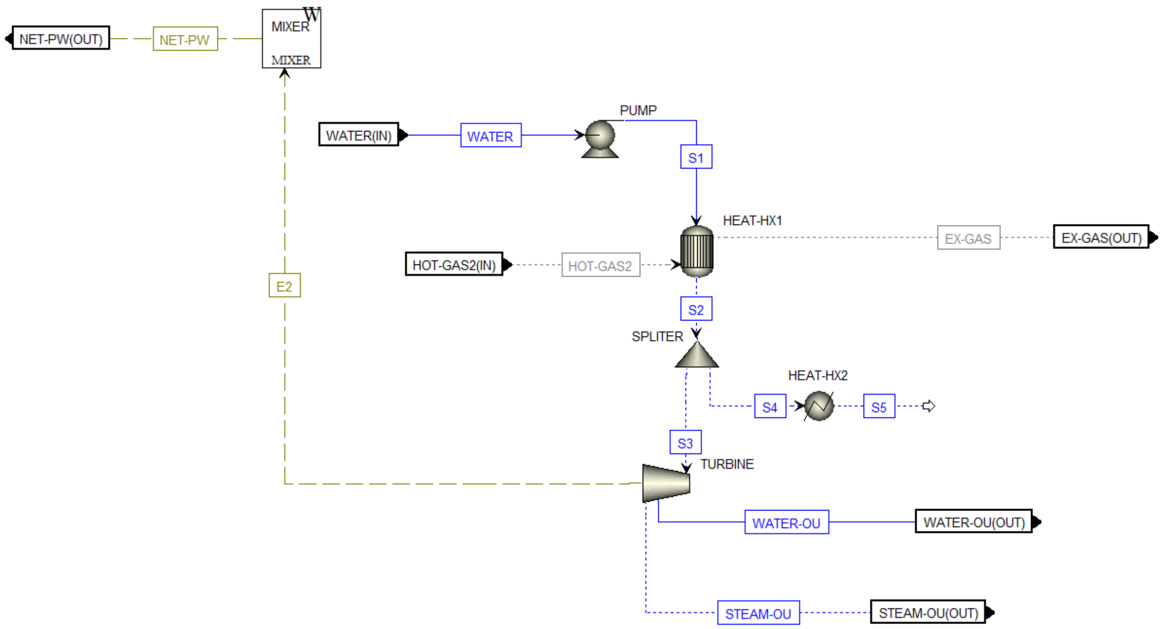

Figure S4. Scheme of the hierarchy BR2, the energy generation stage, under the reference scenario.

Source: Own elaboration.

Figure S5 shows the simulation scheme of the hierarchy BR2 under the alternative system, in which the total generated steam (139,426 kg/h at 526 °C and 50 atm) flows through a turbine to generate electricity. The exhaust steam leaving the turbine (at 362 °C and 15 atm) can cover the internal heat requirements of the sugarcane mill (95 MW_{heat}). Unlike other simulation blocks, the thermodynamic model of the heat exchanger was changed to ASME 1967 steam tables correlation (STEAM-TA) for its cold side.

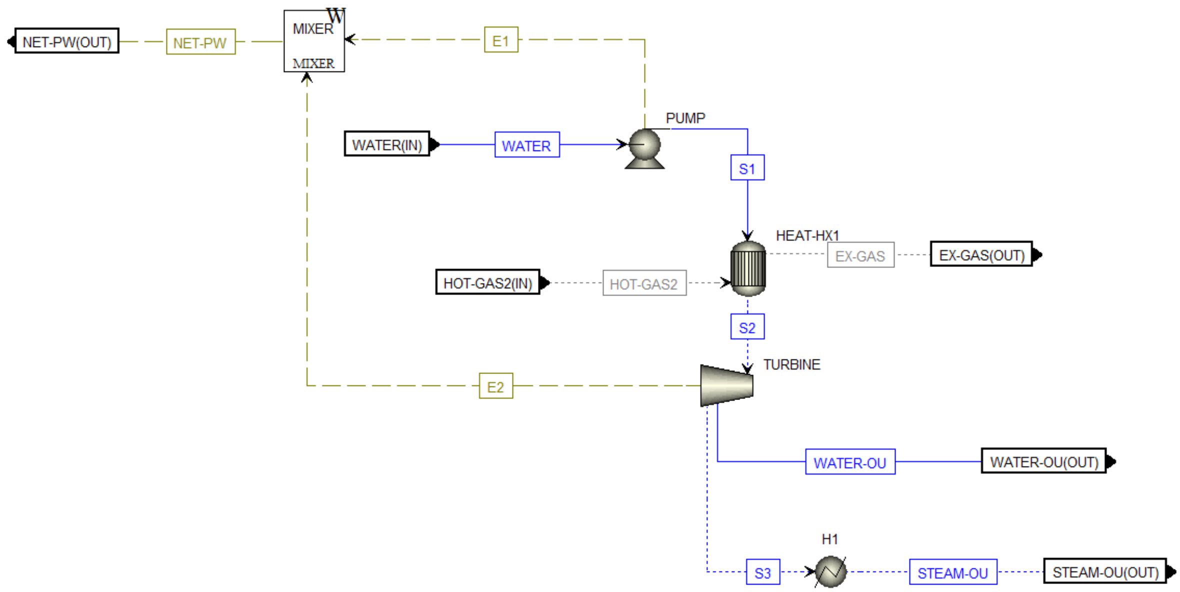

Figure S5. Scheme of the hierarchy BR2, the energy generation stage, under the alternative scenario.

Source: Own elaboration.

Table S6 shows the input data of the blocks simulated in this hierarchy BR2 and their results. Unless otherwise is specified, these conditions are the same for the reference and alternative scenarios.

Table S6. Input data and results of the blocks in the hierarchy BR2.

Equipment	Simulation block	Input data	Results
PUMP	Pump	Discharge pressure: 15 atm under the reference scenario and 50 atm under the alternative scenario Efficiency: 0.85	Electricity: 66.31 kW
HEAT-HX1	HeatX	Hot outlet stream temperature: 280 °C under the reference scenario and 170 °C under the alternative scenario	Outlet temperature: 280 °C under the reference scenario and 170 °C under the alternative scenario Heat duty: 106.7 MW under the reference scenario and 123 MW under the alternative scenario
TURBINE	Compr	Discharge pressure: 0.0835 atm under the reference scenario and 15 atm under the alternative scenario Isentropic efficiency: 0.85 Mechanical efficiency: 0.97	Net work required: -5 MW under the reference scenario and -12 MW under the alternative scenario

Source: Own elaboration.

2. Indicators Data, Assumptions and Calculations

Table S7. Greenhouse Gas Emissions (GHG). Inventory data and Emission factors.

Parameter	Data	Source
Agronomic Phase		
Harvested area (ha)	18,608	[4]
Sugarcane productivity (ton/ha)	74.79	[4]
Bagasse in cane (%)	26	[4]
Seasonal irrigation (%)	95	[5]
Irrigation area (%)	5	[5]
Pumping irrigation (%)	5	[5]
Energy for irrigation (kWh/ha)	219	[5]
Trash burning (% of harvested area)	93	[4]
Dry based matter in trash (%)	0.14	[5,6]
Diesel consumption (L/ha)	131	[5,7]
Nitrogen fertilization (kg/ha)	105	[5]
Proportion of N to N_2O (%)	1	[8]
P_2O_5 fertilization (kg/ha)	51	[5]
K_2O fertilization (kg/ha)	153	[5]
CaCO fertilization (kg/ha)	1,000	[5]
Pesticides (kg/ha)	2	[5]
Transport Phase		
Diesel consumption (L/ton)	2.2	[5]
Industrial Phase		
Sugarcane crushed (ton/year)	1,342,080	[4]
Industrial productivity (% of sugar/ton of cane)	10.79	[4]
Industrial productivity (kg of sugar/ha)	8,069.7	Calculated
Sugar production (kg/ton of cane)	107.9	Calculated
Molasses production (ton)	45,635	[4]
Fuel oil consumption (L/ton of cane)	0.6	[4]
Electricity from the grid on Reference System (kWh/year)	101,940	[4]
Lubricants (kg/ha)	0.77	[5]
Lime (kg/ha)	65.81	[9]
Molasses cost (USD/ton)	4.6	[10]

Table S7. Greenhouse Gas Emissions (GHG). Inventory data and Emission factors (Cont.).

Parameter	Data	Source
Sugar cost (USD/ton)	46.4	[10]
Bagasse cost (USD/ton)	1	Questionaries
Proportion of electricity used in sugarcane preparation and grinding (%)	54	[11]
Emission factors		
Emissions from electrical grid ($kgCO_{2e}$/kWh)	0.527	[12]
Cane trash burning emission factor ($kgCO_{2e}$/kg of dry matter)	0.0828	[7]
Diesel emission factor ($kgCO_{2e}$/L)	3.31*	[13]
Nitrogen fertilizer emission factor ($kgCO_{2e}$/kg)	5.88	[14]
P_2O_5 fertilizer emission factor ($kgCO_{2e}$/kg)	1	[14]
K_2O fertilizer emission factor ($kgCO_{2e}$/kg)	0.5761	[14]
CaO fertilizer emission factor ($kgCO_{2e}$/kg)	0.1295	[5]
Pesticides emission factor ($kgCO_{2e}$/kg)	10.97	[14]
Fuel oil emission factor ($kgCO_{2e}$/L)	3.3**	[14]
Bagasse emission factor ($kgCO_{2e}$/kg)	0.025	[6]
Lubricants emission factor ($kgCO_{2e}$/kg)	0.947	[5]
Lime emission factor ($kgCO_{2e}$/kg)	1.03	[5]

*Considers 43.1 MJ/kg of LHV and 832 kg/m^3 of density.

**Considers 39.3 MJ/L of LHV

Table S8. Emission of particulate matter. Inventory data and Emission factors.

Parameter	Data	Source
Agronomic Phase		
Harvested area (ha)	18,608	[4]
Sugarcane productivity (ton/ha)	74.79	[4]
Bagasse in cane (%)	26	[4]
Trash burning (% of harvested area)	93	[4]
Emission factors		
PM trash burning emission factor (kg/kg of trash)	1.81	[15]
PM bagasse burning emission factor (kg/ton of bagasse)	0.63	[16]
PM fueloil g/kWh	2.61	[17]

Table S9. Direct jobs. Inventory data.

Parameter	Data	Source
Agronomic Phase		
Jobs on the sugarcane cultivation (temporary for 3 months)	3000	Questionaries
Days of work in sugarcane cultivation (days/year)	90	Questionaries
Jobs on the sugarcane harvest (temporary for 5 months)	4167	Questionaries
Days of work in sugarcane harvest (days/year)	150	Questionaries
Transport Phase		
Jobs on the sugarcane transport (temporary for 5 months)	492	Questionaries
Days of work in sugarcane transportation (days/year)	150	Questionaries
Industrial Phase		
Jobs in the Zafra period (temporary for 5 months)	636	Questionaries
Days of work in the Zafra period (days/year)	154	Questionaries
Jobs in the Reparation period (temporary for 7 months)	456	Questionaries
Days of work in the Reparation period (days/year)	211	Questionaries
Cane processed (ton/year)	1,342,080	[4]
Electricity generation Reference System (kWh/ton of cane)	15.11	[4]
Electricity generation Alternative System (kWh/ton of cane)	36.21	Calculated (simulation data)

Table S10. Net Present Value (NPV).

Technical data	unit	CBS	EBS	Sources
Capacity	MW	5	12	Simulation data
Electricity produced	kWh/y	21,031,022	50,389,774.1	Calculated (simulation data)
		Economic Data		
Investment Cost				
Power generation system cost per unit	USD2018/ MW		1,200,000	[18]
Power generation system cost	USD2017	5,874,865.4	14,099,676.9	Calculated (simulation data)
		Operation and Maintenance Costs		
Water quantity	L/y	590,749,688	590,749,688	Questionaries
Unit cost of water	USD2017/ L	2	2	Questionaries
Cost of water used per year	USD2017	29,921.5	29,921.5	* Simulation.
O&M Cost (Percentage of cost of capital per year)		0		
Workforce	USD2017/y	253,000	359,260	[19]
Equipment maintenance - boiler and turbines	USD2017/y	176,246	422,990.3	[20,21]

C. Questionnaire

Social Indicator that aply to all LCA stages: agricultural, transport, industrial and end-use.	
	Incidences of occupational injuries
1	How often are there absences due to accidents or illnesses? by stage (# accidents/year)
The following questions apply only to the Industrial stage	
Social Indicators	
	Employment
2	How many workers oversee the cogeneration system (total for all shifts)?
3	How many shifts are there?
	Average annual income per capita
4	How much is the annual per capita income of the repair staff? ($)
	Training level
5	How many of the repair staff have a bachelor's degree or higher?
Environmental Indicators	
6	**Water Consumption (L/ton sugarcane)**
7	Is water used for sugarcane washing?
8	Amount of water used for sugarcane washing (m/ton sugarcane)
9	Is any reagent, chemical added?
10	If so, what is the reagent?
11	Specify the quantity of this reagent, chemical (L or kg/ton sugarcane).
12	Does the wastewater receive any treatment? Which one?
13	Where the wastewater goes?
14	Do you have a wastewater treatment plant?
	Water treatment plant
15	With which water quality standards does your treated water comply?
16	What type of treatment plant is it?
	Specify the parameters of the water input to the WWTP
17	Litres of treated water (L/s)
18	Total suspended solids (mg/L)
19	Chemical Oxygen Demand (mg/L)
20	Total Nitrogen (mg/L)
	Specify the following discharge parameters, outlet of the WWTP
21	Litres of water discharged (L/s)
22	Total Suspended Solids (mg/L)
23	Chemical Oxygen Demand (mg/L)
24	Total Nitrogen (mg/L)
25	% Removal

26	Residual sludge (kg/ton sugarcane)
27	How much electrical energy is consumed at the WWTP? (kWh/L treated water)
	Water for steam generation
28	Amount of water used for steam generation (L/ton sugarcane)
Electricity consumption	
29	Is disaggregated electricity consumption available?
	Specify by process
30	Milling (kWh/ton sugarcane)
31	Process (kWh/ton sugarcane)
32	Process (kWh/ton sugarcane)
Air Emissions (from bagasse combustion in a boiler)	
33	Is PROY-NOM-70-SEMARNAT-07 being followed?
34	Does this sugarmill comply with the emission limits?
35	What is the nominal thermal capacity of the boiler? (GJ/h)
36	Specify the parameters related to the combustion of ton of bagasse sugarcane bagasse
37	Particulate Matter (mg/m)
38	Carbon monoxide (ppmv)
39	Sulphur dioxide (ppmv)
40	Nitrogen oxides (ppmv)
Ash management	
41	How much ash is generated? (ton/ton bagasse)
42	What type of treatment does it receive?
43	Is it transported to a confinement site?
44	Distance to the confinement site (km/ton ash)
45	Type of vehicle used for transport (trailer, truck, van, etc.)
46	Total capacity (tons)
47	Type of fuel used (diesel or gasoline or other)
48	Trips made to transport one ton of ash per ton of bagasse
49	Are ashes transported to a treatment site?
50	Distance to treatment site (km/ton ash)
51	Type of vehicle used for transport (trailer, truck, van, etc.)
52	Capacity (ton)
53	Type of fuel used (diesel or gasoline or other)
54	Trips made to transport one ton of ash per ton of bagasse
Bagasse sludge	
54	How much bagasse sludge is generated? (ton/ton of bagasse)
55	What type of treatment does it receive?
56	Is it transported to a site?
57	Distance to treatment site (km/ton bagasse sludge)

58	Type of vehicle used for transport
59	Capacity (ton)
60	Type of fuel used (diesel or gasoline or other). Trips made (ton)
61	Trips made to transport one ton of bagasse sludge per ton of bagasse
Boiler operation data	
	Current boiler operating conditions
62	Operating time (hours/year)
63	Amount of bagasse burned (ton/hour)
64	Amount of electricity generated from one ton of bagasse (kWh/ton bagasse)
65	Voltage and current of this electricity (V) and (A)
66	Combustion temperature (°C)
67	Pressure (bar)
68	Gas flow (kg/hour)
69	Does the steam directly go to turbines for electricity generation? Specify quantity or what percentage
70	Goes to other turbomachinery or to Heat in the sugar manufacturing process? Specify quantity and what percentages
Steam turbine	
71	Initial conditions of the steam entering the turbine
72	Final conditions of the steam exiting the turbine
73	Is the steam output condensed or is it released to the atmosphere?
Economic Indicators	
74	What is the selling price of molasses? ($/ton molasses)
75	What is the selling price of sugar? ($/ton sugar)
76	What is the selling price of bagasse? ($/ton bagasse)
77	What is the selling price of sugarcane juice? ($/ton juice)
78	How much do you pay to CFE for each kWh? ($/kWh)
79	How much do you pay for fuel oil? ($/litre)
80	How much do you pay for water? ($/m)
81	What is the operation and maintenance cost of the cogeneration system (including boiler)? ($/ton sugarcane)
82	Do you know the amount of investment in a cogeneration system like the one you currently have?
83	What is the cost at which the mill buys sugarcane from producers?
84	What is the cost of handling the bagasse before it is used in the boiler?

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