

Life Cycle Analysis of Succinic Acid Production in the Brazilian Biorefinery Context

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1. Inventories

1.1. Scenario 1

Developed from the simulation of the process. It uses sugarcane juice as carbon source for the fermentative process conducted by *E. coli* microorganisms. Table S1 presents data referring to the production stage.

Table S1. Inventory of the industrial stage of SA production from sugarcane.

INPUTS		
Air	5,80E+01	kg
Sugarcane Juice {BR}	1,56E+01	kg
Water, decarbonised {BR} market for water, decarbonised Cut-off, U	7,40E+01	kg
Sodium hydroxide, without water, in 50% solution state {GLO} market for Cut-off, U	1,56E-02	kg
Zeolite, powder {GLO} market for Cut-off, U	4,30E-04	kg
Ammonia, anhydrous, liquid {RoW} market for ammonia, anhydrous, liquid Cut-off, U	1,51E-02	kg
Electricity, high voltage {BR-South-eastern grid} treatment of bagasse, from sugarcane, in heat and power co-generation unit, 6400kW thermal Cut-off, U	1,19E+00	kWh
Heat, district or industrial, other than natural gas {BR-Southern grid} treatment of bagasse, from sugarcane, in heat and power co-generation unit, 6400kW thermal Cut-off, U	1,18E+01	MJ
OUTPUTS		
Succinic acid {BR} Sugarcane first generation process	1,00E+00	kg

The sugarcane juice inventory was adapted from OCAMPO BATTLE (2021) considering as input the sugarcane production inventory present in Ecoinvent for the southeast region of Brazil. The inputs and outputs can be seen in Table S2.

Table S2. Inventory of sugarcane juice production.

INPUTS		
Sugarcane {BR-SP} sugarcane production Cut-off, U	1,14E+00	kg
Water, decarbonised {BR} market for water, decarbonised Cut-off, U	3,43E-02	kg
Transport, freight, lorry >32 metric ton, EURO1 {BR} market for transport, freight, lorry >32 metric ton, EURO1 Cut-off, U	3,42E-0	tkm
Electricity, medium voltage {BR-South-eastern grid} market for electricity, medium voltage Cut-off, U	1,82E+01	Wh
OUTPUTS		
Sugarcane Juice {BR}	1,00E+00	kg

To analyze the impacts of the upstream, fermentation and downstream stages of the sugarcane production process, the inputs were divided to generate 3 inventories corresponding to the stages (table S3).

Table S3. Distribution of inputs for each stage of the industrial process for producing SA from sugar cane.

INPUTS	Upstream	Fermentation	Downstream	
Air	2,76E+00	-	5,52E+01	kg
Water, decarbonised {BR} market for water, decarbonised Cut-off, U	4,71E+01	1,03E+01	1,66E+01	kg
Sugarcane Juice {BR}	1,56E+01	-	-	kg
Sodium hydroxide, without water, in 50% solution state {GLO} market for Cut-off, U	-	-	1,56E-02	kg
Ammonia, anhydrous, liquid {RoW} market for ammonia, anhydrous, liquid Cut-off, U	-	1,51E-02	-	kg
Zeolite, powder {GLO} market for Cut-off, U	-	4,30E-04	-	kg
Electricity, high voltage {BR-South-eastern grid} treatment of bagasse, from sugarcane, in heat and power co-generation unit, 6400kW thermal Cut-off, U	0,00E+00	1,19E+00	3,98E-02	kWh
Heat, district or industrial, other than natural gas {BR-Southern grid} treatment of bagasse, from sugarcane, in heat and power co-generation unit, 6400kW thermal Cut-off, U	1,00E+00	7,75E+00	3,01E+00	MJ

1.2. Scenario 2

Table S4. Inventory of the industrial step of SA production from sorghum.

INPUTS		
Water, unspecified natural origin, BR-Southern grid	1,29E+00	m ³
Grain sorghum, at farm	1,66E+00	kg
Glucose {GLO} market for glucose Cut-off, U	1,30E-02	kg
Water, decarbonised {BR} market for water, decarbonised Cut-off, U	1,67E+00	kg
Water, ultrapure {RoW} market for water, ultrapure Cut-off, U	2,53E+01	kg
Ammonia, anhydrous, liquid {RoW} market for ammonia, anhydrous, liquid Cut-off, U	4,10E-01	kg
Heat, from steam, in chemical industry {RoW} steam production, as energy carrier, in chemical industry Cut-off, U	1,48E+01	MJ
Electricity, medium voltage {BR-South-eastern grid} market for electricity, medium voltage Cut-off, U	2,67E+00	kWh
Transport, freight, lorry >32 metric ton, EURO1 {BR} market for transport, freight, lorry >32 metric ton, EURO1 Cut-off, U	4,98E-02	tkm
OUTPUTS		
Succinic Acid {BR} Sorghum first generation process	1,00E+00	kg
Ammonium sulfate	1,49E+00	kg
EMISSIONS		
To air		
Organic substances, unspecified	2,00E-03	kg
Carbon monoxide	1,50E-02	kg
Nitrogen oxides	5,00E-03	kg
Particulates	5,00E-03	kg
Ammonia	1,72E-04	kg
Lead	5,20E-06	kg
To water		
Sulfuric acid	8,06E-05	kg
Waste water	1,10E+01	kg
Residual		
Waste, organic	1,22E+00	kg

The inventory (Table S5) of the agricultural stage of sorghum production was adapted for the southeastern region of Brazil.

Table S5. Inventory of the agricultural stage of sorghum production in Brazil.

INPUTS		
Carbon dioxide, in air	3,92E-03	kg
Transformation, to arable land, unspecified use	3,39E-03	m ²
Occupation, arable land, unspecified use	3,38E-03	m ² a
Urea, as N {GLO} market for Cut-off, U	1,40E-01	kg
Limestone, crushed, washed {RoW} market for limestone, crushed, washed Cut-off, U	1,56E-02	kg
Maize seed, organic, at farm {GLO} market for Cut-off, U	5,90E+00	kg
Glyphosate {GLO} market for Cut-off, U	1,04E+00	kg
Atrazine {GLO} market for Cut-off, U	9,88E-01	kg
Pesticide, unspecified {GLO} market for Cut-off, U	2,01E-02	kg
Diesel {BR} market for diesel Cut-off, U	1,98E-01	kg

Electricity, high voltage {BR-South-eastern grid} market for electricity, high voltage Cut-off, U	3,33E+00	kWh
OUTPUTS		
Sorghum Grain, at farm	1,00E+00	ton
EMISSIONS		
To air		
Carbon dioxide, fossil	9,28E-01	kg
Carbon dioxide, land transformation	4,14E-03	kg
Dinitrogen monoxide	9,68E-01	kg
Nitrogen oxides	1,16E+00	kg
Ammonia	3,33E+00	kg
NMVOC, non-methane volatile organic compounds	6,75E-02	kg
Carbon monoxide, fossil	1,22E-01	kg
Sulfur dioxide	2,28E-02	kg
Methane, fossil	2,91E-03	kg
Benzene	1,64E-04	kg
Cadmium	2,25E-07	kg
Chromium	1,13E-06	kg
Copper	3,84E-05	kg
Nickel	1,58E-06	kg
Zinc	2,25E-05	kg
Benzopyrene, methyl-	6,75E-08	kg
Selenium	2,25E-08	kg
Benz[a]anthracene,12-methyl-	1,80E-06	kg
Benzo(a)fluoranthene	1,13E-06	kg
Cresol	4,52E-06	kg
Dibenz(a,h)anthracene	2,25E-07	kg
Fluoranthene	1,01E-05	kg
Phenanthrene	5,62E-05	kg
To water		
Cadmium	4,66E-11	kg
Copper	7,57E-08	kg
Zinc	8,67E-08	kg
Lead	1,01E-09	kg
Chromium	1,48E-07	kg
To field		
Cadmium	4,66E-06	kg
Copper	7,57E-04	kg
Zinc	8,67E-04	kg
Lead	1,01E-05	kg
Chromium	1,48E-03	kg
Glyphosate	1,04E+00	kg
Atrazine	9,88E-01	kg
Thiamethoxam	2,01E-02	kg
Lambda-cyhalothrin	1,58E-02	kg

1.3. Scenario 3

The inventory referring to the 3rd scenario does not consider obtaining the apple pomace, since it is residue from another process. Thus, considering only the industrial stage.

Table S6. Inventory of the industrial stage of second-generation SA production in Brazil

INPUTS		
Tap water {BR} market for tap water Cut-off, U	2,29E-02	kg
Glucose {GLO} market for glucose Cut-off, U	5,93E-02	kg
Corn steep liquor/kg/RNA	1,48E-02	kg
Carbon dioxide, in chemical industry {GLO} market for carbon dioxide, in chemical industry Cut-off, U	1,25E-02	kg
Chemical, inorganic {GLO} market for chemical, inorganic Cut-off, U	2,50E-01	kg
Sodium chloride, powder {GLO} market for Cut-off, U	2,51E-01	kg
Sulfuric acid {RoW} market for sulfuric acid Cut-off, U	8,31E-01	kg
Natural gas liquids {GLO} market for Cut-off, U	3,12E-01	kg
Enzymes {GLO} market for enzymes Cut-off, U	1,35E-02	kg
Chemical, organic {GLO} market for Cut-off, U	4,70E-02	kg
Electricity, medium voltage {BR-South-eastern grid} market for electricity, medium voltage Cut-off, U	7,87E-02	kWh
Transport, freight, lorry >32 metric ton, EURO1 {BR} market for transport, freight, lorry >32 metric ton, EURO1 Cut-off, U	5,40E-02	tkm
OUTPUTS		
Succinic Acid {BR} Apple pomace second generation	1,00E+00	kg
EMISSIONS		
to air		
Methane	3,56E-05	kg
Carbon monoxide	5,33E-04	kg
Ethanol	2,68E-06	kg
Nitrogen monoxide	8,89E-06	kg
Sulfur oxides	9,79E-06	kg
Particulates	1,78E-06	kg
Nitrogen oxides	3,56E-04	kg
to water		
Waste water	2,41E-02	kg
Residual		
Waste, unspecified	8,85E-01	kg

1.4. Scenario 4

Inventory (Table S7) adapted from ecoinvent for the Brazilian scenario considering the chemical route of SA production from maleic anhydride.

Table S7. Inventory of SA production from the chemical route

INPUTS		
Water, unspecified natural origin, BR-Southern grid	0,01809	m ³
Maleic Anhydride {BR} production by catalytic oxidation of benzene	8,74E-01	kg
Hydrogen, gaseous {BR} hydrogen production, gaseous, petroleum refinery operation Cut-off, U	1,80E-02	kg
Water, decarbonised {BR} market for water, decarbonised Cut-off, U	1,87E-01	kg
Metal catalyst for catalytic converter {GLO} market for metal catalyst for catalytic converter Cut-off, U	4,97E-05	kg
Nitrogen, liquid {RoW} market for Cut-off, U	1,90E-02	kg
Electricity, medium voltage {BR-Southern grid} market for electricity, medium voltage Cut-off, U	4,16E-01	kWh
Heat, district or industrial, natural gas {GLO} market group for Cut-off, U	2,35E+00	MJ
OUTPUTS		
Succinic Acid {BR} Chemical route	1,00E+00	kg
EMISSIONS		
To air		
Carbon dioxide, fossil	7,45E-02	kg
Hydrogen	8,98E-04	kg
Nitrogen, atmospheric	1,90E-02	kg
Water/m3	1,67E-02	m ³
To water		
Maleic anhydride	2,19E-03	kg
Water, BR-South-eastern grid	1,67E-02	m ³
To technologic sphere		
Wastewater, average {RoW} market for wastewater, average Cut-off, U	2,74E-06	m ³

Inventory (Table S8) adapted from ecoinvent for the Brazilian scenario considering the production of maleic anhydride from the catalytic oxidation of benzene.

Table S8. Inventory maleic anhydride production.

INPUTS		
Water, cooling, unspecified natural origin, BR-Southern grid	1,46E-02	kg
Water, river	7,66E-04	kg
Water, well	7,39E-04	kg
Benzene {GLO} market for Cut-off, U	1,02E+00	kg
Chemical factory {GLO} market for Cut-off, U	3,56E-10	kg
Tap water {BR} market for tap water Cut-off, U	2,32E-01	kg
Electricity, medium voltage {BR-South-eastern grid} market for electricity, medium voltage Cut-off, U	5,34E-01	kWh
OUTPUTS		
Maleic Anhydride {BR} production by catalytic oxidation of benzene	1	kg

2. Figures

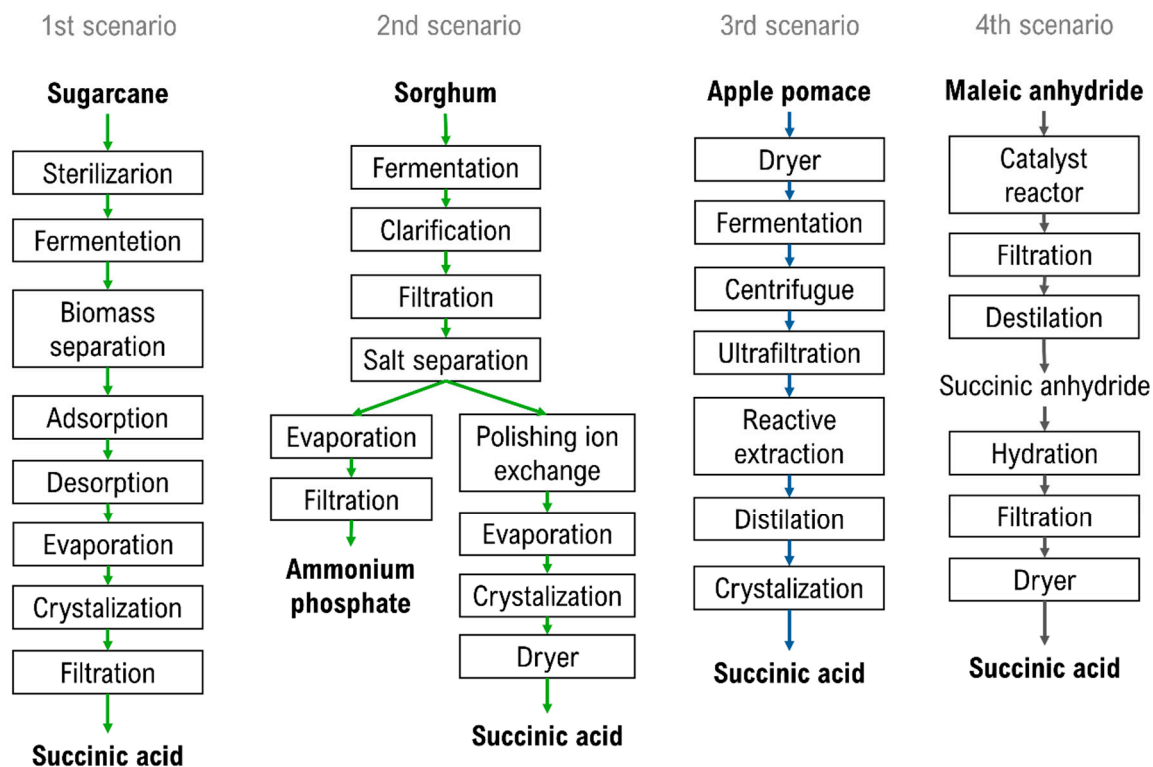


Figure S1. Flowchart of succinic acid production from: first generation sugarcane; first generation sorghum; second generation apple pomace and chemical route maleic anhydride.