Technical, Environmental, and Process Safety Assessment of Acetone-Butanol-Ethanol Fermentation of Cassava Residues

Samir Meramo [1,2,*], Arturo Gonzalez-Quiroga [3] and Angel Gonzalez-Delgado [4,*]

[1] Novo Nordisk Foundation Center for Biosustainability, Technical University of Denmark, Building 220, Kemitorvet Kgs., 2800 Lyngby, Denmark

[2] Grupo de Investigación de Ingeniería, Innovación y Productividad, Industrial Engineering Program, Cra. 50# 31, Cartagena 130005, Colombia

[3] UREMA Research Unit, Mechanical Engineering Department, Universidad del Norte, Barranquilla 25138, Colombia

[4] Nanomaterials and Computer-Aided Process Engineering Research Group (NIPAC), Chemical Engineering Department, University of Cartagena, Consulado Avenue, St. 30 #48-152, Cartagena 130015, Colombia

* Correspondence: samhur@biosustain.dtu.dk (S.M.); agonzalezd1@unicartagena.edu.co (A.G.-D.); Tel.: +45-91670914 (S.M.)

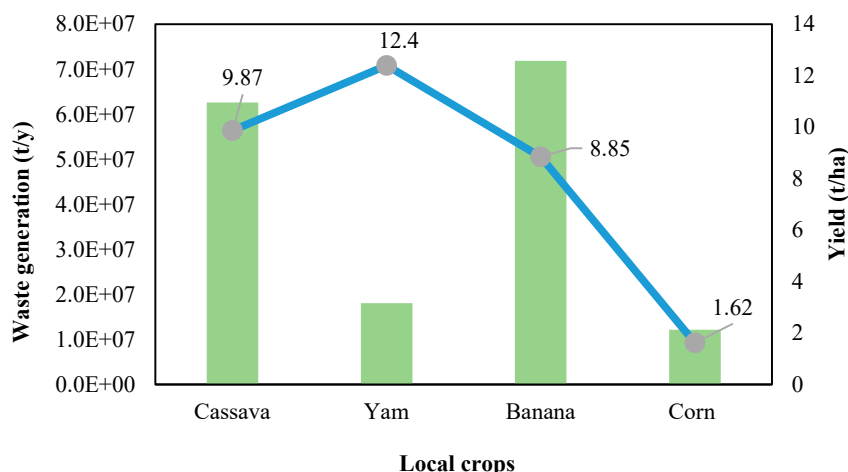### Data on agricultural residues in Bolivar

Figure S1. Available agricultural residues and yields of local crops in Bolivar. Source: [25]

ABE process upstream and downstream data

Table S1. Gathered data for upstream processing simulation in route 1

Step	Operating variable	Value	Reference
	Particle size (mm)	5	[27]
	Temperature (°C)	190	[28]
	Pression (atm)	12.2	[29]
	% Solids	0.42	
Pretreatment	Acid concentration (%wt)	0.0011	[28]
	Water mass flow (t/h)	638.34	Estimated
	Water supply (t/h)	552.55	Estimated
	Acid mass flow (t/h)	9.97	Estimated

	NH$_3$ concentration (%wt)	1.1	[28]
	NH$_3$ mass flow rate (t/h)	0.02	Estimated
	Duty (GJ/h)	1,384.14	Estimated
	Reactions	$(\text{Xylan})_n + n\text{H}_2\text{O} \rightarrow n\text{Xylose}$ $(\text{Xylan})_n \rightarrow n\text{Furfural} + 2\text{H}_2\text{O}$ $(\text{Glucan})_m + m\text{H}_2\text{O} \rightarrow m\text{Glucose}$ $(\text{Glucan})_m + \frac{1}{2}n\text{H}_2\text{O} \rightarrow m\text{Cellobiose}$ $\text{Acetate} \rightarrow \text{Acetic acid}$ $\text{Lignin} \rightarrow \text{Soluble lignin}$ $\text{H}_2\text{SO}_4 + \text{Ca(OH)}_2 \rightarrow \text{CaSO}_4 \cdot 2\text{H}_2\text{O}$	[27]
Hydrolysis	Temperature (°C)	45	[28]
	Pressure (atm)	1.66	[29]
	% Moisture	88.90%	[34]
	% NaOH	2.0	
	Solid to liquid ratio	1:10	
	Solid mass flow (t/h)	176.61	[41]
	NaOH mass flow (t/h)	35.92	
	Water supply (t/h)	1,790.08	
	Duty (GJ/h)	102.70	Estimated
	Reactions	$(\text{Glucan})_m + m\text{H}_2\text{O} \rightarrow m\text{Glucose}$ $\text{Cellobiose} + m\text{H}_2\text{O} \rightarrow 2\text{Glucose}$	[46]
Fermentation	Temperature (°C)	37	[41]
	Pressure (atm)	1	
	Moisture (%)	80%	[27]
	Duty (GJ/h)	-172.48	Estimated
	Reactions	$\text{Glucose} \rightarrow \text{Butanol} + 2\text{CO}_2 + \text{H}_2\text{O}$ $\text{Glucose} + \text{H}_2\text{O} \rightarrow \text{Acetone} + 3\text{CO}_2 + 4\text{H}_2$ $\text{Glucose} \rightarrow 2\text{Ethanol} + 2\text{CO}_2$ $\text{Glucose} \rightarrow \text{Butyric acid} + 2\text{CO}_2 + 2\text{H}_2$ $\text{Glucose} \rightarrow 3\text{ Acetic acid}$ $6\text{Xylose} \rightarrow 5\text{Butanol} + 10\text{CO}_2 + 5\text{H}_2\text{O}$ $\text{Xylose} \rightarrow \text{Acetone} + 2\text{CO}_2 + 2\text{H}_2$ $3\text{Xylose} \rightarrow 5\text{Ethanol} + 5\text{CO}_2$ $2\text{Xylose} \rightarrow 5\text{ Acetic acid}$	[53, 55]

Table S2. Gathered data for upstream processing simulation in route 2

Step	Operating variable	Value	Reference
Pretreatment	Temperature (°C)	195	[63]
	Pressure (atm)	36	
	Water/biomass ratio	2.56	[64]
	Steam/biomass ratio	0.6054	
	Water flow	829.33	Estimated

	Steam supply (t/h)	216.41	Estimated
	Water supply (t/h)	612.92	Estimated
	Reactions	See Table S1	[27]
Hydrolysis	Temperature (°C)	45	
	Pressure (atm)	1.66	[27]
	% Moisture	88.90%	[29]
	% NaOH	2.0	
	Solid to liquid ratio	1:10	
	Solid flow (t/h)	211.01	[31]
	Liquid flow (t/h)	2110.14	
	NaOH mass flow (t/h)	42.2	
	Water supply (t/h)	2104.1	
	Reactions	See Table S1	[34]
Fermentation	Temperature (°C)	37	[41]
	Pressure (atm)	1	
	Moisture (%)	80%	[27]
	Reactions	See Table S1	[46]

Downstream processing description

Table S3. Gathered data for downstream processing simulation in route 1

Step	Operating variable	Value	Reference
Gas stripping (GS-1)	Number of stages	10	[63]
	Reflux ratio (mass)	3	
	Feed stage	1	
	Pressure (atm)	1	
Beer column (BC-1)	Number of stages	4	[34]
	Reflux ratio (mass)	1.5	
	Feed stage	2	
	Pressure (atm)	1	
	Distillate-to-feed ratio	0.836	
	Condenser heat duty (GJ/h)	331.05	Estimated
	Reboiler heat duty (GJ/h)	502.89	
Acetone column (AC-1)	Number of stages	20	
	Reflux ratio (mass)	15	
	Feed stage	3	
	Pressure (atm)	0.5	Estimated
	Distillate-to-feed ratio	0.156	

	Operating variable	Value	Reference
	Condenser heat duty (GJ/h)	168.21	
	Reboiler heat duty (GJ/h)	32.92	
Ethanol column (ET-1)	Number of stages	50	Estimated
	Reflux ratio (mass)	30	
	Feed stage	8	
	Pressure (atm)	0.1	
	Distillate-to-feed ratio	0.011	
	Condenser heat duty (GJ/h)	33.72	
	Reboiler heat duty (GJ/h)	49.97	
Butanol column (BTC-1)	Number of stages	12	Estimated
	Reflux ratio (mass)	5	
	Feed stage	9	
	Pressure (atm)	1	
	Bottoms-to-feed ratio	0.63	
	Condenser heat duty (GJ/h)	90.10	
	Reboiler heat duty (GJ/h)	121.90	

First, a beer column separates substantial amounts of water and other impurities from the ABE-rich stream. Next, the acetone-rich stream is subjected to distillation and further condensation at 98.1%wt purity. The bottom of the acetone distillation column (rich in ethanol and butanol) is sent to a distillation column for ethanol separation from butanol. The recovered ethanol forms a homogeneous azeotrope with water, broken using a molecular sieve to obtain a purity of 99.82%wt. The bottom stream of the ethanol column contains a butanol-water mixture that forms a heterogeneous azeotrope. Water removal from this mixture commonly includes columns with internal decanters [64]. Based on that configuration, the butanol-water is sent to a liquid-liquid extraction unit (decanter) to collect some organic phase rich in butanol that is withdrawn as reflux into a distillation column for purification [75]. The final product is finally condensed with 99.39%wt purity. Route 2 also uses double-effect distillation columns to separate butanol and acetone; however, reactive distillation is incorporated to break the azeotrope. This biobutanol purification technology consists of an extractant agent, i.e., ethylene oxide, reacting with water from the azeotropic system to produce ethylene glycol [76]. This route provides butanol at 99.9%wt., acetone at 99.06%wt, and ethylene glycol at 98.85%wt. Table S4 summarizes the operational parameters of downstream units in route 2.

Table S4. Gathered data for downstream processing simulation in route 2

Step	Operating variable	Value	Reference
Gas stripping (GS-1)	Number of stages	10	[63]
	Reflux ratio (mass)	3	
	Feed stage	1	
	Pressure (atm)	1	
Distillation column (DT-1)	Number of stages	10	[34]
	Reflux ratio (mass)	1	
	Feed stage	5	
	Pressure (atm)	1	
	Bottoms-to-feed ratio	0.635	Estimated
	Condenser heat duty (GJ/h)	33.62	

	Reboiler heat duty (GJ/h)	55.23	
Reactive column 1 (RC-1)	Number of stages	10	[76]
	Reflux ratio (mass)	12	
	Feed stage	5	
	Pressure (atm)	1	
	Distillate-to-feed ratio	0.546	
	Condenser heat duty (GJ/h)	294.98	Estimated
	Reboiler heat duty (GJ/h)	258.17	
Reactive column 2 (RC-2)	Number of stages	10	[76]
	Reflux ratio (mass)	10	
	Feed stage	9	
	Pressure (atm)	1	
	Distillate-to-feed ratio	0.44	
	Condenser heat duty (GJ/h)	77.80	Estimated
	Reboiler heat duty (GJ/h)	42.19	
Distillation column (DT-2)	Number of stages	12	[77]
	Reflux ratio (mass)	5	
	Feed stage	9	
	Pressure (atm)	1	Estimated
	Bottoms-to-feed ratio	0.63	
	Condenser heat duty (GJ/h)	90.10	
	Reboiler heat duty (GJ/h)	121.90	
Distillation column (DT-3)	Number of stages	15	[77]
	Reflux ratio (mass)	10	
	Feed stage	15	
	Pressure (atm)	0.3	
	Bottoms-to-feed ratio	0.116	Estimated
	Condenser heat duty (GJ/h)	78.34	
	Reboiler heat duty (GJ/h)	76.14	

Table S5. Gathered data for downstream processing simulation in route 1

Step	Operating variable	Value	Reference
Gas stripping (GS-1)	Number of stages	10	[63]
	Reflux ratio (mass)	3	
	Feed stage	1	
	Pressure (atm)	1	
Beer column (BC-1)	Number of stages	4	[34]
	Reflux ratio (mass)	1.5	
	Feed stage	2	
	Pressure (atm)	1	
	Distillate-to-feed ratio	0.836	
	Condenser heat duty (GJ/h)	331.05	Estimated
	Reboiler heat duty (GJ/h)	502.89	
Acetone column (AC-1)	Number of stages	20	
	Reflux ratio (mass)	15	
	Feed stage	3	
	Pressure (atm)	0.5	Estimated

	Distillate-to-feed ratio	0.156	
	Condenser heat duty (GJ/h)	168.21	
	Reboiler heat duty (GJ/h)	32.92	
Ethanol column (ET-1)	Number of stages	50	Estimated
	Reflux ratio (mass)	30	
	Feed stage	8	
	Pressure (atm)	0.1	
	Distillate-to-feed ratio	0.011	
	Condenser heat duty (GJ/h)	33.72	
	Reboiler heat duty (GJ/h)	49.97	
Butanol column (BTC-1)	Number of stages	12	Estimated
	Reflux ratio (mass)	5	
	Feed stage	9	
	Pressure (atm)	1	
	Bottoms-to-feed ratio	0.63	
	Condenser heat duty (GJ/h)	90.10	
	Reboiler heat duty (GJ/h)	121.90	

First, a beer column separates substantial amounts of water and other impurities from the ABE-rich stream. Next, the acetone-rich stream is subjected to distillation and further condensation at 98.1%wt purity. The bottom of the acetone distillation column (rich in ethanol and butanol) is sent to a distillation column for ethanol separation from butanol. The recovered ethanol forms a homogeneous azeotrope with water, broken using a molecular sieve to obtain a purity of 99.82%wt. The bottom stream of the ethanol column contains a butanol-water mixture that forms a heterogeneous azeotrope. Water removal from this mixture commonly includes columns with internal decanters [76]. Based on that configuration, the butanol-water is sent to a liquid-liquid extraction unit (decanter) to collect some organic phase rich in butanol that is withdrawn as reflux into a distillation column for purification [27]. The final product is finally condensed with 99.39%wt purity. Route 2 also uses double-effect distillation columns to separate butanol and acetone; however, reactive distillation is incorporated to break the azeotrope. This biobutanol purification technology consists of an extractant agent, i.e., ethylene oxide, reacting with water from the azeotropic system to produce ethylene glycol [77]. This route provides butanol at 99.9%wt., acetone at 99.06%wt, and ethylene glycol at 98.85%wt. Table S6 summarizes the operational parameters of downstream units in route 2.

Table S6. Gathered data for downstream processing simulation in route 2

Step	Operating variable	Value	Reference
Gas stripping (GS-1)	Number of stages	10	[75]
	Reflux ratio (mass)	3	
	Feed stage	1	
	Pressure (atm)	1	
Distillation column (DT-1)	Number of stages	10	[34]
	Reflux ratio (mass)	1	
	Feed stage	5	
	Pressure (atm)	1	Estimated

|			
	Bottoms-to-feed ratio	0.635	
	Condenser heat duty (GJ/h)	33.62	
	Reboiler heat duty (GJ/h)	55.23	
Reactive column 1 (RC-1)	Number of stages	10	[79]
	Reflux ratio (mass)	12	
	Feed stage	5	
	Pressure (atm)	1	
	Distillate-to-feed ratio	0.546	
	Condenser heat duty (GJ/h)	294.98	Estimated
	Reboiler heat duty (GJ/h)	258.17	
Reactive column 2 (RC-2)	Number of stages	10	
	Reflux ratio (mass)	10	
	Feed stage	9	[79]
	Pressure (atm)	1	
	Distillate-to-feed ratio	0.44	
	Condenser heat duty (GJ/h)	77.80	Estimated
	Reboiler heat duty (GJ/h)	42.19	
Distillation column (DT-2)	Number of stages	12	[80]
	Reflux ratio (mass)	5	
	Feed stage	9	
	Pressure (atm)	1	Estimated
	Bottoms-to-feed ratio	0.63	
	Condenser heat duty (GJ/h)	90.10	
	Reboiler heat duty (GJ/h)	121.90	
Distillation column (DT-3)	Number of stages	15	[80]
	Reflux ratio (mass)	10	
	Feed stage	15	
	Pressure (atm)	0.3	
	Bottoms-to-feed ratio	0.116	Estimated
	Condenser heat duty (GJ/h)	78.34	
	Reboiler heat duty (GJ/h)	76.14	

Process simulation of Route 1

As shown in Figure S1-a), the simulation of route 1 was divided into four main hierarchy blocks: pretreatment (PT-1), hydrolysis (HD-1), fermentation (FER-1), and purification (SEP-1). The first hierarchy block includes both mechanical and dilute-acid pretreatments. The simulation flowsheet for this block is displayed in Figure S1-b). The cassava residues (stream 1) enter the gyratory crusher CH-1 for particle size reduction at a cut-off size to solids outlet diameter ratio of 1.7. The acid pretreatment takes place in the reactor RX-1 by adding steam (stream 11), water (stream 7), and sulfuric acid solution (stream 6). The stream leaving the pretreatment reactor is sent to a flash vessel FC-1 to remove the excess water and small quantities of acetic acid and furfural. Then, it passes through the filter FT-1 to separate water-soluble sugars (stream 17) from hydrolysate slurry (stream 19). The latter is then neutralized with ammonia (stream 20) in the IOX-1, while the dissolved sugar stream is directly sent to fermentation. The detoxification is completed in the reactor RX-2, where calcium hydroxide (stream 25) reacts with sulfuric acid to produce calcium disulfate. The resulting stream is subjected to filtration in the FT-2, which feedbacks the liquid outlet stream

into the process. Finally, the pretreated biomass (stream 30) is collected from the separator FT-3 and sent to the hierarchy block of hydrolysis.

The enzymatic hydrolysis of pretreated biomass (Figure S1-c) was modeled using two reactors: one for lignin solubilization (ST-1) and one for glucose production (RX-3). The cellulase (stream 31) was mixed with the biomass before entering the first reactor. The outlet stream of the ST-1 reactor included solubilized lignin removed in the SP-1 unit, portions of cellulase, and traces of xylose. The stream leaving the separator enters the second reactor RX-3 for cellulose conversion into glucose by the action of the enzyme (stream 39). The 75% reactor outlet is fed into the FER-1 hierarchy block (stream 41), while the remaining (stream 42) is sent back to mix with the cellulase. This process was simulated using the reactor RX-4 by adding the fermentation broth (stream INNOC) and water (stream 45). Figure S1-d depicts the simulation flowsheet for cassava residues fermentation. The ABE products and by-products are obtained from fermentation reactions and sent to the downstream processing (SEP-1 block).

The outlet of the fermentation reactor (stream 46) enters the *in-situ* gas stripper GS-1, in which light components (stream 47) such as ABE products are separated from undesired compounds (stream 48), including cellulose, ash, hemicellulose, calcium sulfate, and furfural. Due to the azeotrope formation between ethanol/water and butanol-water, double-effect distillation columns were added to the downstream simulation (Figure S1-e). The following equipment is a two-outlet flash separator CD-1 modeled to collect 95%wt. CO_2, while the bottom stream passes through the beer column BC-1. The stream leaving the top of this column contains desired products, and the bottom stream is mainly water and traces of acetic acid and butyric acid. The acetone is separated from the mixture (stream 54) in the distillation column AC-1 followed by the flash separator CD-2 with three outlets: acetone-H_2-CO_2 (stream 58), water (stream 59), and acetone (stream 60). The bottom stream of AC-1 is pumped to the distillation column ET-1 to recover ethanol from the mixture and collect a butanol-rich stream. The stream rich in ethanol (stream 64) passes through the molecular sieve MS-1 to separate water and increase the purity of the product. Then, the butanol-rich stream (stream 65) enters the decanter DC-1 to remove the excess water (stream 74). The purification of butanol continues in the distillation column BTC-1, where butanol is recovered from the bottom (stream 79), and the top outlet (stream 76) is sent back to the decanter.

a)
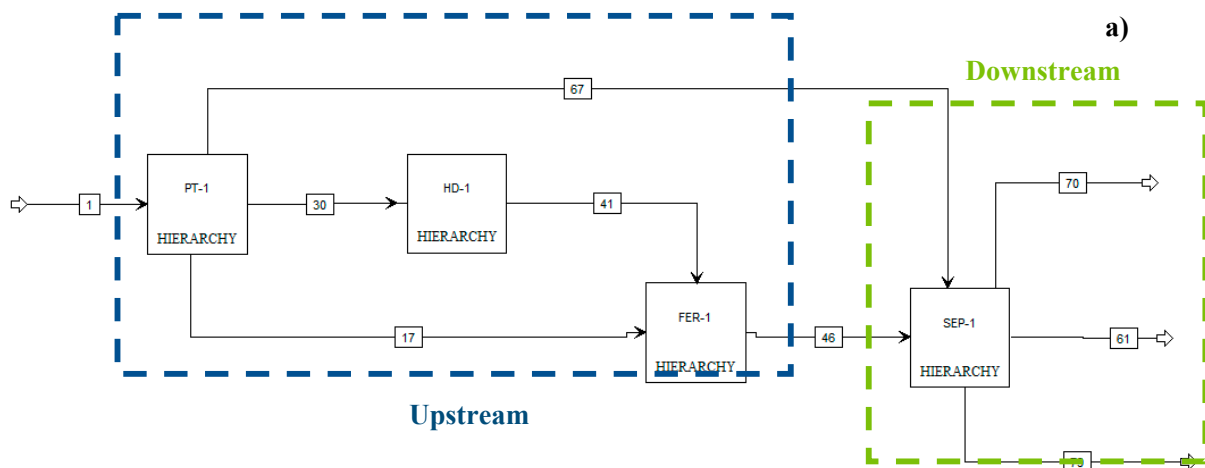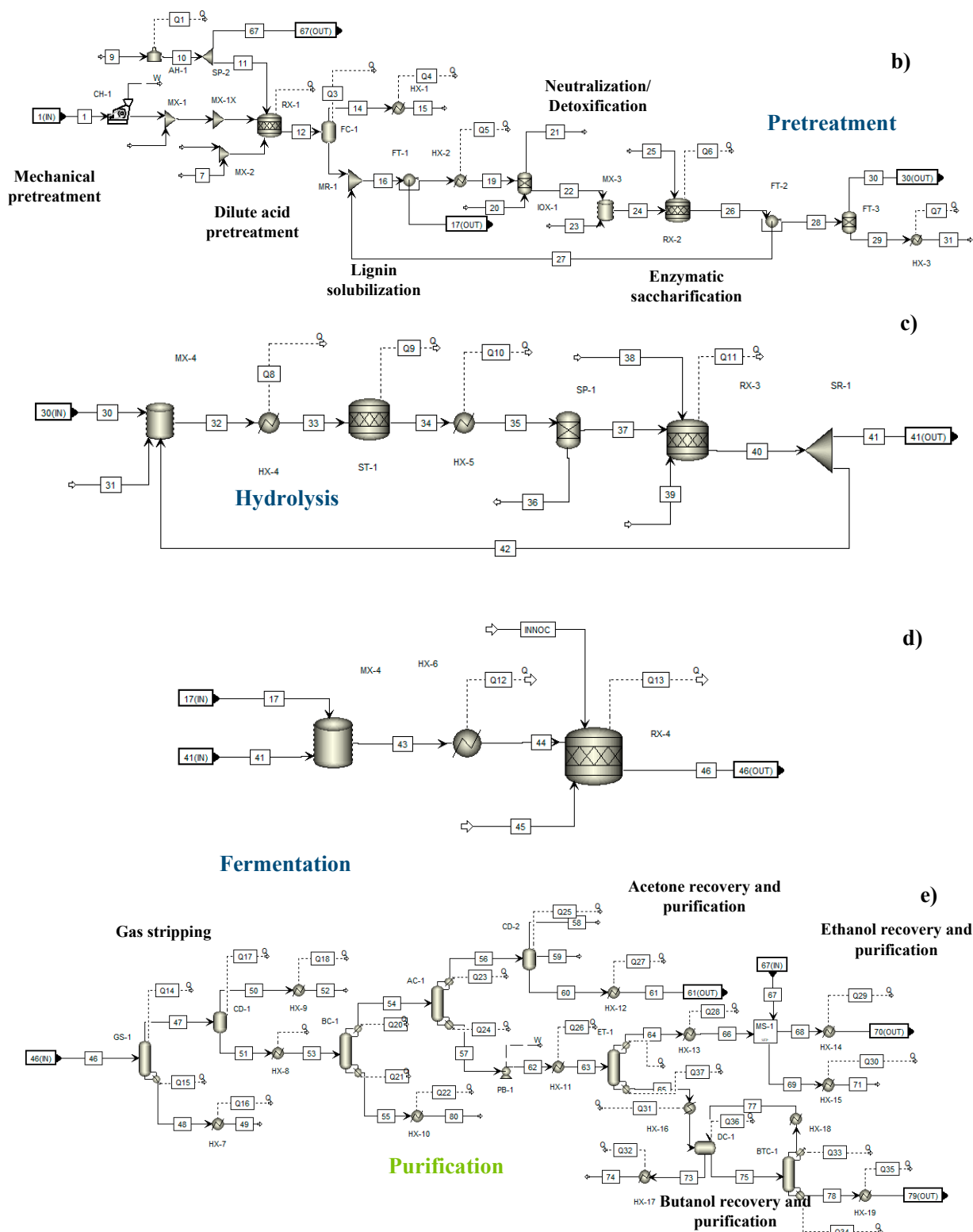
Figure S2. Simulation flowsheet for route 1: a) hierarchy blocks of upstream and downstream processing, b) pretreatment, c) hydrolysis, d) fermentation and e) purification.
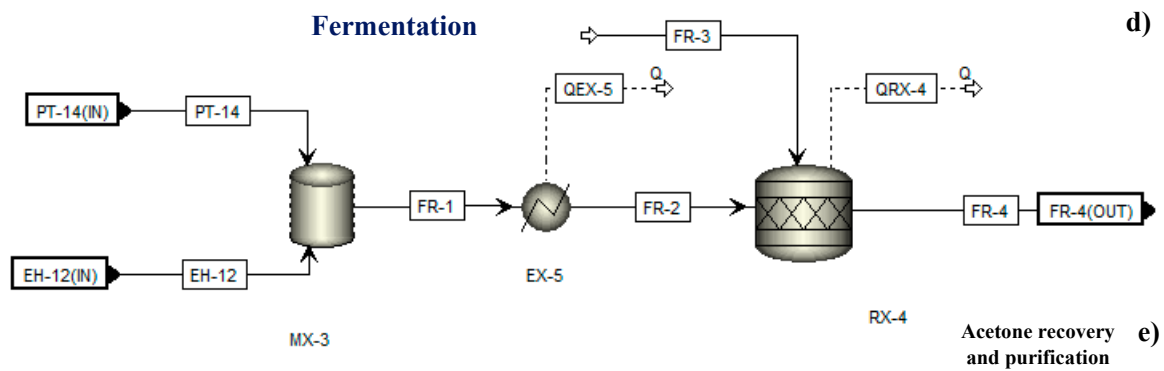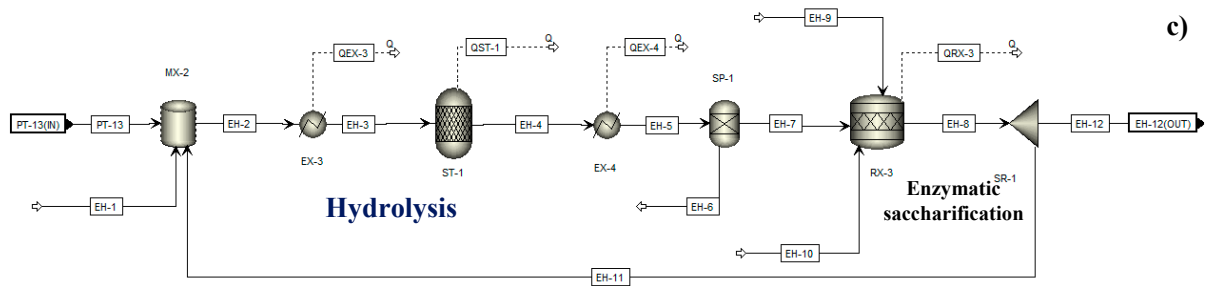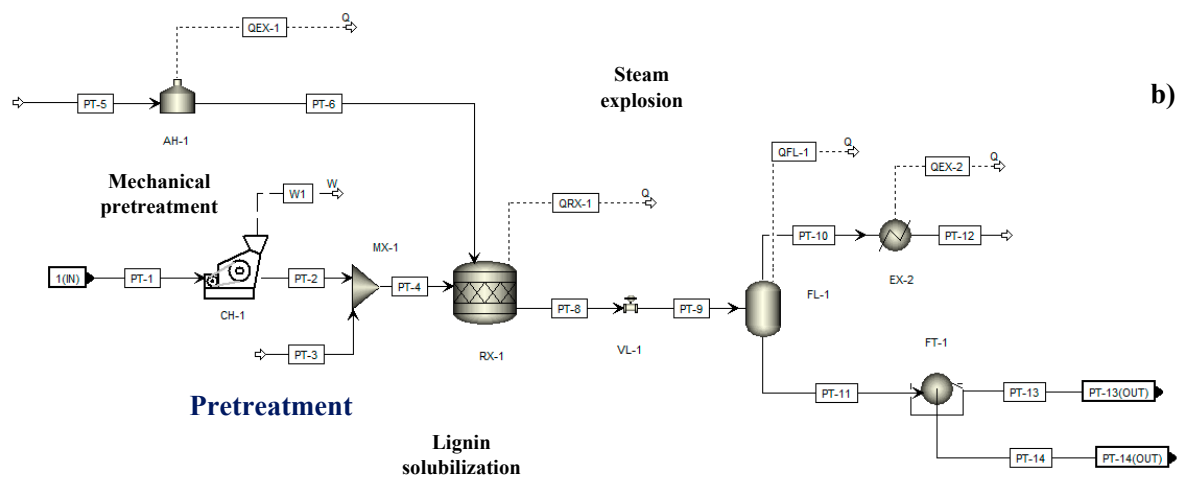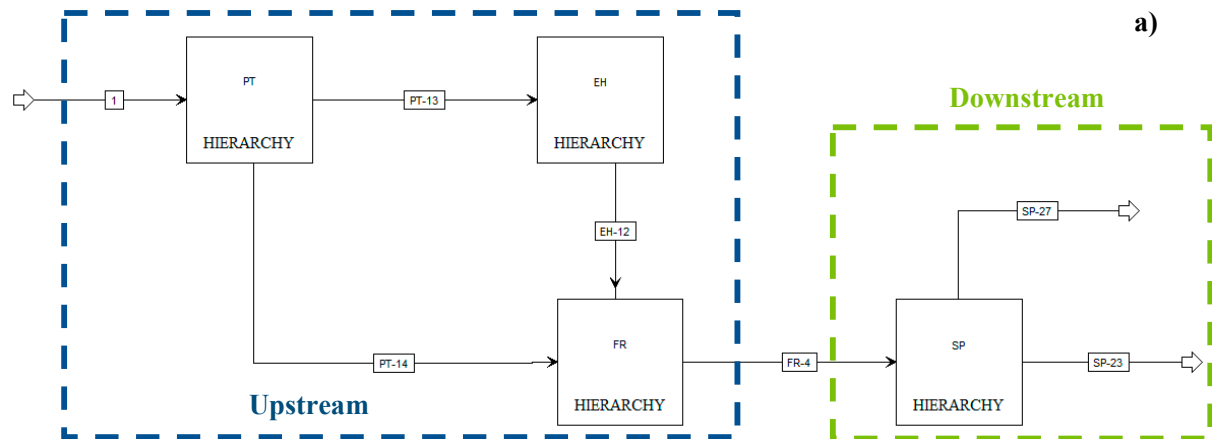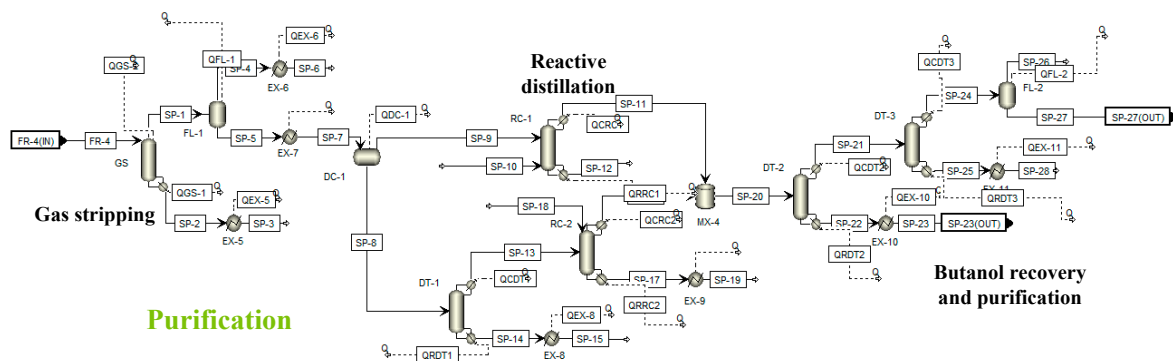
Process simulation Route 2

As depicted in Figure S2-a), the hierarchy blocks of this route are like route 1 with the following labels: pretreatment (PT), hydrolysis (EH), fermentation (FR), and purification (SP). The simulation flowsheet of the biomass pretreatment during upstream processing is shown in Figure S2-b. The biomass (stream PT-1) enters the gyratory crusher CH-1 for particle size reduction and is then sent to the reactor RX-1 for the steam explosion. In this reactor, steam (stream PT-6) reacts with the cellulose and hemicellulose to produce glucose and xylose. The outlet stream passes through the flash vessel FL-1 to remove water excess (stream PT-12) and the acetic acid formed during pretreatment. The stream leaving the bottom of the separator is fed into the filter FT-1 to separate the liquid containing soluble sugars (stream PT-14) directly sent to fermentation. The solid outlet from the filter (stream PT-13) is subjected to enzymatic hydrolysis.

Figure S2-c) shows the simulation results for enzymatic hydrolysis of the pretreated biomass. The stream PT-13 is mixed with enzyme solution (stream EH-1) before entering the reactor ST-1. Like route 1, lignin solubilization occurs in this reactor, followed by its removal (stream EH-6) in the separator SP-1. The stream free of lignin (stream EH-7) passes through the reactor RX-3 along with water (stream EH-9) and enzyme (stream EH-10) to produce glucose. Then, the reaction products (stream EH-12) are mixed with the water-soluble sugars (stream PT-14), as depicted in the simulation of the FR hierarchy block (Figure S2-d). During fermentation, the broth (stream FR-3) is added to the reactor RX-4, where sugars are converted to ABE products. The stream leaving this reactor FR-4 is sent to the purification of desired products (Figure S2-e).

The simulation of the purification process starts with separating cellulose, hemicellulose, lignin, and ashes (stream SP-3) from the fermentation products in the gas stripping (GS). The top outlet of this column contains the by-product carbon dioxide, which leaves the system in the stream SP-6 after flash vessel FL-1. The bottom stream of FL-1 (stream SP-5) passes through the decanter DC-1, and two outlet streams are obtained: water-rich (stream SP-8) and desired products-rich (stream SP-9). The water content from stream SP-8 is removed in the distillation column DT-1, while the remaining components are sent to the reactive distillation column RC-2. In this column, the ethylene-oxide (stream SP-18) reacts with water leading to the outlet of ethylene-glycol (stream SP-17) from the bottom. This ethylene-glycol is also obtained from the reactive distillation column RC-1 (stream SP-12) after adding ethylene-oxide (stream SP-10) to the stream SP-9. Ethylene oxide also reacts with ethanol in the ethoxylation reaction. However, the influence of this reaction is not considered in the reactive distillation system since experimental kinetic data have shown that this reaction happens at significantly lower rates than the hydration rate of ethylene oxide because of the absence of a catalyst for this reaction [81].

The resulting stream from mixing the top outlets of both columns RC-1 and RC-2 is sent to the distillation column DT-2, where the separation of ABE products begins. Butanol is collected from the bottom of this column (stream 23), while the top stream containing acetone and ethanol is subjected to distillation in column DT-3. The acetone-rich stream (stream 24) feeds into the flash vessel FL-2 to reach a high-purity product (stream 27), while the ethanol mixture (SP-18) is considered outlet waste.

a)

Downstream

Upstream

b)

Steam explosion

Mechanical pretreatment

Pretreatment

Lignin solubilization

c)

Hydrolysis

Enzymatic saccharification

Fermentation

d)

Acetone recovery and purification

e)

Figure S3. Simulation flowsheet for route 2: a) hierarchy blocks of upstream and downstream processing, b) pretreatment, c) hydrolysis, d) fermentation and e) purification.

Simulation validation

This study validated the simulation results by calculating the accuracy of main product properties from simulation and literature. As summarized in Table S7, the simulated properties of biobutanol achieved high accuracy (>98%) for RVP, boiling point, density, and standard enthalpy of vaporization. This analysis was also performed for other components, obtaining similar accuracy levels. These results confirmed the proper selection of the thermodynamic package during process simulation and validated the data provided by the software.

Table S7. Estimation of relevant properties for biobutanol using Aspen Plus

Biobutanol properties	This work	Other contributions	Accuracy (%)	Reference
Reid vapor pressure-RVP (kPa)	5.20	5.30[+]	98.1	[82]
Boiling point (°C)	118. 75	117.20[±]	98.7	[83]
Density @ 25°C(kg/L)	0.81	0.81[§]	99.6	[84]
Kinematic viscosity@ 25°C(cSt)	3.20	3.70[§]	86.5	[84]
Standard enthalpy of vaporization (kJ/kg)	722	716[*]	99.2	[85]
Cetane number	21.40	17[§]	74.1	[83]

Table S8. Estimation of relevant properties for ethanol using Aspen Plus

Biobutanol properties	This work	Other contributions	Accuracy (%)
Liquid vapor pressure (kPa)	5.89	5.89[+]	100
Boiling point (°C)	78.29	78.37[±]	99.8
Density @ 25°C(kg/L)	0.804	0.79[*]	99.6
Kinematic viscosity@ 25°C(cSt)	1.47	1.20[*]	77.75
Standard enthalpy of vaporization (MJ/mol)	42.84	42.41[*]	98.98

[+] [86]; [±] [87]; [*] [88]

Table S9. Estimation of relevant properties for acetone using Aspen Plus

Biobutanol properties	This work	Other contributions	Accuracy (%)
Liquid vapor pressure (kPa)	24.71	24.59[+]	99.50
Boiling point (°C)	56.29	56.00[±]	99.80
Density @ 25°C(kg/L)	0.804	0.79*	99.60
Kinematic viscosity@ 25°C(cSt)	0.40	0.39*	97.43
Standard enthalpy of vaporization (MJ/mol)	31.47	31.27*	99.36

[+][86]; [±][89]; *[90]

Table S10. Operating data of main process streams for route 1

Stream	1	3	4	6	8	9
T (°C)	28	28	28	28	28	28
P (atm)	1	1	1	1	1	1
Mass flowrate (kg/h)	353895.51	343721.46	697616.97	10386.32	20754.58	228310.50
Components						
GLUCAN	0.4040	0.0000	0.2050	0.0000	0.0000	0.0000
XYLAN	0.1313	0.0000	0.0666	0.0000	0.0000	0.0000
LIGNIN	0.1212	0.0000	0.0615	0.0000	0.0000	0.0000
ASH	0.0505	0.0000	0.0256	0.0000	0.0000	0.0000
AACID	0.0505	0.0000	0.0256	0.0000	0.0000	0.0000
WATER (Liquid)	0.2424	1.0000	0.6157	0.0400	0.5196	1.0000
Water (Vapor)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
XYLOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
GLUCOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SULFU-01	0.0000	0.0000	0.0000	0.9600	0.4804	0.0000
FURFU-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CELLO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-02	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CELLULASE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MICROORG	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BUTANOL	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ACETONA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ETHANOL	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CARBO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N-BUT-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S10. Operating data of main process streams for route 1 (continue)

Stream	14	15	20	21	25	34
T (°C)	103	28	28	40	28	90
P (atm)	1	1	1	1	1	1
Mass flowrate (kg/h)	599305.98	599305.98	24.75	7570.92	490.24	3662366.51
Components						

GLUCAN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0382
XYLAN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0025
LIGNIN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0115
ASH	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AACID	0.0241	0.0241	0.0000	0.0565	0.0000	0.0000
WATER (Liquid)	0.0000	0.9728	0.0000	0.7553	0.0000	0.8287
Water (Vapor)	0.9728	0.0000	0.0000	0.0000	0.0000	0.0054
XYLOSE	0.0004	0.0004	0.0000	0.0000	0.0000	0.1123
GLUCOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SULFU-01	0.0000	0.0000	0.0000	0.1849	0.0000	0.0000
FURFU-01	0.0027	0.0027	0.0000	0.0000	0.0000	0.0000
CELLO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON-01	0.0000	0.0000	1.0000	0.0033	0.0000	0.0000
CALCI-02	0.0000	0.0000	0.0000	0.0000	1.0000	0.0000
CALCI-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
CELLULASE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0011
MICROORG	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BUTANOL	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ACETONA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ETHANOL	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CARBO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N-BUT-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S10. Operating data of main process streams for route 1 (continue)

Stream	40	41	INNOC	47	58	61
T (°C)	28	45	28	81	37	28
P (atm)	1	1.66	1	1	1	1
Mass flowrate (kg/h)	2245433.17	561358.29	11578.08	229576.34	982.58	15888.85
Components						
GLUCAN	0.0062	0.0062	0.0000	0.0000	0.0000	0.0000
XYLAN	0.0041	0.0041	0.0000	0.0000	0.0000	0.0000

Component						
LIGNIN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ASH	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AACID	0.0000	0.0000	0.0000	0.0014	0.0000	0.0000
WATER (Liquid)	0.7368	0.7368	0.0000	0.3069	0.0015	0.0048
Water (Vapor)	0.0088	0.0088	0.0000	0.0000	0.0000	0.0000
XYLOSE	0.2434	0.2434	0.0000	0.0000	0.0000	0.0000
GLUCOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SULFU-01	0.0000	0.0000	0.0000	0.0003	0.0000	0.0000
FURFU-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CELLO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-02	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-01	0.0007	0.0007	0.0000	0.0000	0.0000	0.0000
CELLULASE	0.0000	0.0000	1.0000	0.0000	0.0000	0.0000
MICROORG	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BUTANOL	0.0000	0.0000	0.0000	0.1906	0.0001	0.0030
ACETONA	0.0000	0.0000	0.0000	0.0785	0.5598	0.9810
ETHANOL	0.0000	0.0000	0.0000	0.0051	0.0021	0.0058
CARBO-01	0.0000	0.0000	0.0000	0.4059	0.4363	0.0053
N-BUT-01	0.0000	0.0000	0.0000	0.0009	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000	0.0103	0.0002	0.0000

Table S10. Operating data of main process streams for route 1 (continue)

Stream	66	70	71	78	79	80
T (°C)	110	28	28	118	28	28
P (atm)	1	1	1	1	1	1
Mass flowrate (kg/h)	993.15	828.90	1419.96	36126.69	36126.69	21662.27
Components						
GLUCAN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
XYLAN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
LIGNIN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ASH	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

AACID	0.0000	0.0000	0.0000	0.0006	0.0006	0.0118
WATER (Liquid)	0.1486	0.0017	0.9873	0.0001	0.0001	0.9871
Water (Vapor)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0001
XYLOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
GLUCOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SULFU-01	0.0002	0.0000	0.0001	0.0014	0.0014	0.0000
FURFU-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CELLO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-02	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CELLULASE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MICROORG	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BUTANOL	0.0176	0.0000	0.0123	0.9939	0.9939	0.0000
ACETONA	0.0004	0.0000	0.0003	0.0000	0.0000	0.0000
ETHANOL	0.8332	0.9983	0.0000	0.0000	0.0000	0.0000
CARBO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N-BUT-01	0.0000	0.0000	0.0000	0.0039	0.0039	0.0011
HYDROGEN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S11. Operating data of main process streams for route 2

Stream	PT-1	PT-4	PT-5	PT-11	PT-12	PT-14
T (°C)	28	28	28	115	28	115
P (atm)	1	1	1	1	1	1
Mass flowrate (kg/h)	320829	592717	778905	234189	1137433	42892
Components						
GLUCAN	0.4040	0.2187	0.0000	0.5109	0.0000	0.0279
XYLAN	0.1313	0.0711	0.0000	0.0397	0.0000	0.0022
LIGNIN	0.1212	0.0656	0.0000	0.1661	0.0000	0.0091
ASH	0.0505	0.0273	0.0000	0.0692	0.0000	0.0038
AACID	0.0505	0.0273	0.0000	0.0008	0.0141	0.0037
WATER (Liquid)	0.2424	0.5899	1.0000	0.0314	0.9815	0.1403

Water (Vapor)	0.0000	0.0000	0.0000	0.1348	0.0033	0.6022
XYLOSE	0.0000	0.0000	0.0000	0.0431	0.0000	0.1924
GLUCOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SULFU-01	0.0000	0.0000	0.0000	0.0001	0.0011	0.0003
FURFU-01	0.0000	0.0000	0.0000	0.0041	0.0000	0.0183
CELLO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-02	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CELULASA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
LYE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BUTANOL	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ACETONA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ETHANOL	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CARBO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N-BUT-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ETHY-1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ETHY-2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S11. Operating data of main process streams for route 2 (continue)

Stream	EH-1	EH-4	EH-6	EH-9	EH-10	FR-1
T (°C)	28	90	28	28	28	46.32416688
P (atm)	1	1	1	1	1	1
Mass flowrate (kg/h)	1945762	3766593	2836113	1241868	362	586069
Components						
GLUCAN	0.0000	0.0340	0.0000	0.0000	0.0000	0.0075
XYLAN	0.0000	0.0098	0.0000	0.0000	0.0000	0.0159
LIGNIN	0.0000	0.0102	0.0136	0.0000	0.0000	0.0007
ASH	0.0000	0.0170	0.0000	0.0000	0.0000	0.0276
AACID	0.0000	0.0000	0.0000	0.0000	0.0000	0.0003
WATER (Liquid)	0.9803	0.8124	0.9711	1.0000	0.0000	0.6651

Water (Vapor)	0.0000	0.0059	0.0001	0.0000	0.0000	0.0534
XYLOSE	0.0000	0.1002	0.0017	0.0000	0.0000	0.2276
GLUCOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SULFU-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
FURFU-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0013
CELLO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-02	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-01	0.0000	0.0003	0.0000	0.0000	1.0000	0.0006
CELULASA	0.0197	0.0102	0.0135	0.0000	0.0000	0.0000
LYE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BUTANOL	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ACETONA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ETHANOL	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CARBO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
N-BUT-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ETHY-1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ETHY-2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S11. Operating data of main process streams for route 2 (continue)

Stream	FR-2	FR-4	SP-1	SP-4	SP-5	SP-6
T (°C)	37	37	77	3	3	28
P (atm)	1	1	1	1	1	1
Mass flowrate (kg/h)	586069	737076	187007	86357	100651	86357
Components						
GLUCAN	0.0075	0.0060	0.0000	0.0000	0.0000	0.0000
XYLAN	0.0159	0.0126	0.0000	0.0000	0.0000	0.0000
LIGNIN	0.0007	0.0005	0.0000	0.0000	0.0000	0.0000
ASH	0.0276	0.0220	0.0000	0.0000	0.0000	0.0000
AACID	0.0003	0.0029	0.0006	0.0000	0.0010	0.0000
WATER (Liquid)	0.6651	0.6298	0.2504	0.0040	0.4619	0.0040

Component						
Water (Vapor)	0.0534	0.0219	0.0000	0.0000	0.0000	0.0000
XYLOSE	0.2276	0.0005	0.0000	0.0000	0.0000	0.0000
GLUCOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SULFU-01	0.0000	0.0000	0.0001	0.0000	0.0001	0.0000
FURFU-01	0.0013	0.0011	0.0000	0.0000	0.0000	0.0000
CELLO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-02	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-01	0.0006	0.0005	0.0000	0.0000	0.0000	0.0000
CELULASA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
LYE	0.0000	0.1108	0.0000	0.0000	0.0000	0.0000
BUTANOL	0.0000	0.0523	0.2062	0.0013	0.3820	0.0013
ACETONA	0.0000	0.0214	0.0845	0.0205	0.1393	0.0205
ETHANOL	0.0000	0.0014	0.0056	0.0005	0.0100	0.0005
CARBO-01	0.0000	0.1118	0.4406	0.9492	0.0043	0.9492
N-BUT-01	0.0000	0.0016	0.0007	0.0000	0.0013	0.0000
HYDROGEN	0.0000	0.0029	0.0113	0.0245	0.0000	0.0245
ETHY-1	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ETHY-2	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S11. Operating data of main process streams for route 2 (continue)

Stream	SP-9	SP-10	SP-13	SP-15	SP-16	SP-19
T (°C)	80	28	86	28	99	28
P (atm)	1	1	1	1	1	1
Mass flowrate (kg/h)	52995	28615	17394	30262	12607	16045
Components						
GLUCAN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
XYLAN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
LIGNIN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ASH	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AACID	0.0009	0.0000	0.0000	0.0019	0.0000	0.0000
WATER (Liquid)	0.2207	0.0000	0.2650	0.9974	0.0004	0.0000

Component						
Water (Vapor)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
XYLOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
GLUCOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SULFU-01	0.0002	0.0000	0.0002	0.0000	0.0000	0.0002
FURFU-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CELLO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-02	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CELULASA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
LYE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BUTANOL	0.5994	0.0000	0.3843	0.0000	0.5169	0.0105
ACETONA	0.1585	0.0000	0.3235	0.0000	0.4461	0.0001
ETHANOL	0.0117	0.0000	0.0221	0.0000	0.0305	0.0000
CARBO-01	0.0067	0.0000	0.0043	0.0000	0.0060	0.0000
N-BUT-01	0.0019	0.0000	0.0006	0.0007	0.0000	0.0006
HYDROGEN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ETHY-1	0.0000	1.0000	0.0000	0.0000	0.0000	0.0000
ETHY-2	0.0000	0.0000	0.0000	0.0000	0.0000	0.9885

Table S11. Operating data of main process streams for route 2 (continue)

Stream	SP-20	SP-22	SP-23	SP-25	SP-26	SP-27
T (°C)	107	118	28	57	33	33
P (atm)	1	1	1	0.3	1	1
Mass flowrate (kg/h)	53788	37480	37480	1820	684	13804
Components						
GLUCAN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
XYLAN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
LIGNIN	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
ASH	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AACID	0.0007	0.0010	0.0010	0.0004	0.0000	0.0000
WATER (Liquid)	0.0001	0.0000	0.0000	0.0028	0.0000	0.0000
Water (Vapor)	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

XYLOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
GLUCOSE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
SULFU-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
FURFU-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CELLO-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
AMMON-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-02	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CALCI-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
CELULASA	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
LYE	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
BUTANOL	0.7114	0.9990	0.9990	0.4543	0.0000	0.0000
ACETONA	0.2607	0.0000	0.0000	0.0052	0.4960	0.9906
ETHANOL	0.0187	0.0000	0.0000	0.5373	0.0006	0.0019
CARBO-01	0.0080	0.0000	0.0000	0.0000	0.5004	0.0065
N-BUT-01	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
HYDROGEN	0.0000	0.0000	0.0000	0.0000	0.0003	0.0000
ETHY-1	0.0003	0.0000	0.0000	0.0000	0.0027	0.0010
ETHY-2	0.0000	0.0001	0.0001	0.0000	0.0000	0.0000

References

25. Darkwah, K.; Nokes, S.E.; Seay, J.R.; Knutson, B. Mechanistic simulation of batch acetone–butanol–ethanol (ABE) fermentation within situ gas stripping using Aspen PlusTM. Bioprocess Biosyst. Eng. 2018, 41, 1283–1294.

27. Lodi, G.; De Guido, G.; Pellegrini, L.A. Simulation and energy analysis of the ABE fermentation integrated with gas stripping. Biomass Bioenergy 2018, 116, 227–235.

28. Kaymak, D.B. Design and Control of an Alternative Process for Biobutanol Purification from ABE Fermentation. Ind. Eng. Chem. Res. 2019, 58, 1957–1965.

29. Haigh, K.F.; Petersen, A.M.; Gottumukkala, L.; Mandegari, M.; Naleli, K.; Gorgens, J. Simulation and comparison of processes for biobutanol production from lignocellulose via ABE fermentation. Biofuels Bioprod. Biorefining 2018, 12, 1023–1036.

31. Meramo-Hurtado, S.I.; González-Delgado, Á.; Rehmann, L.; Quinones-Bolanos, E.; Mehvar, M. Comparative analysis of biorefinery designs based on acetone-butanol-ethanol fermentation under exergetic, techno-economic, and sensitivity analyses towards a sustainability perspective. J. Clean Prod. 2021, 298, 126761.

34. Carmona-Garcia, E.; Ortiz-Sánchez, M.; Cardona Alzate, C.A. Analysis of the Coffee Cut Stems as Raw Material for the Production of Sugars for Acetone–Butanol–Ethanol (ABE) Fermentation: Techno-Economic Analysis. Waste Biomass Valorization 2019, 10, 3793–3808.

41. Luo, L.; van der Voet, E.; Huppes, G. Biorefining of lignocellulosic feedstock—Technical, economic and environmental considerations. Bioresour. Technol. 2010, 101, 5023–5032.

46. Jin, Q.; Qureshi, N.; Wang, H.; Huang, H. Acetone-butanol-ethanol (ABE) fermentation of soluble and hydrolyzed sugars in apple pomace by Clostridium beijerinckii P260. Fuel 2019, 244, 536–544.

53. Naleli, K. Process Modelling in Production of Biobutanol from Lignocellulosic Biomass via ABE Fermentation. Ph.D. Thesis, Stellenbosch University, Stellenbosch, South Africa, 2016; pp. 63–66.

63. Jones, D.T. Biobutanol. In Biotechnology-Fundamentals in Biotechnology; Encyclopedia of Life Support Systems (EOLSS); EOLSS Publications; United Kingdom; 2009; pp. 98–134.

64. Lapuerta, M.; Ballesteros, R.; Barba, J. Strategies to Introduce n-Butanol in Gasoline Blends. Sustainability 2017, 9, 1–10.

75. Ministerio de Agricultura y Desarrollo Rural . Producción y Rendimiento Nacional por Cultivo; Ministerio de Agricultura y Desarrollo Rural: Bogotá, Colombia, 2018.

76. López-Arenas, T.; Rathi, P.; Ramírez-Jiménez, E.; Sales-Cruz, M. Factors affecting the acid pretreatment of lignocellulosic biomass: Batch and continuous process. Comput. Aided Chem. Eng. 2010, 28, 979–984.

77. Wooley, R.; Ruth, M.; Sheehan, J.; Ibsen, K.; Majdeski, H.; Galvez, A. Lignocellulosic Biomass to Ethanol Process Design and Economics Utilizing Co-Current Dilute Acid Prehydrolysis and Enzymatic

Hydrolysis Current and Futuristic Scenarios; National Renewable Energy Lab. (NREL): Golden, CO, USA, 1999.

78.   El-Naggar, N.E.A.; Deraz, S.; Khalil, A. Bioethanol production from lignocellulosic feedstocks based on enzymatic hydrolysis: Current status and recent developments. Biotechnology 2014, 13, 1–21.

79.   Carvajal, J.C.; Gómez, Á.; Cardona, C.A. Comparison of lignin extraction processes: Economic and environmental assessment. Bioresour. Technol. 2016, 214, 468–476.

80.   Duque, A.; Manzanares, P.; Ballesteros, I.; Ballesteros, M. Steam Explosion as Lignocellulosic Biomass Pretreatment; Elsevier Inc.: Madrid, Spain, 2016.

81.   Chum, H.L.; Douglas, L.J.; Feinberg, D.A.; Schroeder, H.A. Evaluation of Pretreatments of Biomass for Enzymatic Hydrolysis of Cellulose; Solar Energy Research Inst.: Golden, CO, USA, 1985; pp. 1–64.

82.   Ciric, A.R.; Mumtaz, H.S.; Corbett, G.; Reagan, M.; Seider, W.D.; Fabiano, L.A.; Kolesar, D.M.; Widagdo, S. Azeotropic distillation with an internal decanter. Comput. Chem. Eng. 2000, 24, 2435–2446.

83.   An, W.; Lin, Z.; Chen, J.; Zhu, J. Simulation and analysis of a reactive distillation column for removal of water from ethanol-water mixtures. Ind. Eng. Chem. Res. 2014, 53, 6056–6064.

84.   Brandon, B.; Ezike, R. Ethanol and Butanol: Symbiotic partners for a modern fuel. Biofuels Digest 2015, 1.

85.   Anyanwu, R.C.; Rodriguez, C.; Durrant, A.; Ramadan, M.; Olabi, A.G. Micro-Macroalgae Properties and Applications. In Reference Module in Materials Science and Materials Engineering; Elsevier: Amsterdam, The Netherlands, 2018, pp. 1–28.

86.   Bank DD. Vapor Pressure of Ethanol. Available online: http://www.ddbst.com/en/EED/PCP/VAP_C11.php (accessed 4 June 2022).

87.   Mejía, A.; Segura, H.; Cartes, M. Vapor-Liquid Equilibria and Interfacial Tensions of the System Ethanol + 2-Methoxy-2-methylpropane. J. Chem. Eng. Data 2010, 55, 428–434.

88.   Majer, V.; Svoboda, V. Enthalpies of Vaporization of Organic Compounds: A Critical Review and Data Compilation; Boston : Blackwell Scientific Publications, United Kingdom 1985; p. 300.

89.   Engineering Toolbox. Acetone—Thermophysical Properties, Available online: https://www.engineeringtoolbox.com/acetone-2-propanone-dimethyl-ketone-properties-d_2036.html (2018, accessed 4 June 2022).

90.   Ambrose, D.; Ellender, J.H.; Lees, E.B.; Sprake, C.H.; Townsend, R. Thermodynamic properties of organic oxygen compounds XXXVIII. Vapour pressures of some aliphatic ketones. J Chem Thermodyn 1975, 7, 453–472.