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APPENDICES

Appendix A Components Considered in PRO/II

Table A1 List of components considered in PRO/II simulations, the alias used, and the chemical formula

	Component name	Component alias	Chemical Formula
1	Ethanol	ETHANOL	C ₂ H ₆ O
2	Water	WATER	H ₂ O
3	Glucose	C6	C ₆ H ₁₂ O ₆
4	Sucrose	C12	C ₁₂ H ₂₂ O ₁₁
5	Acetic Acid	ACETACID	C ₂ H ₄ O ₂
6	Carbondioxide	CO2	CO ₂
7	Oxygen	O2	O ₂
8	Ammonia	NH3	NH ₃
9	Lactic Acid	LACACID	C ₃ H ₆ O ₃
10	Succinic Acid	SUCCNAC	C ₄ H ₆ O ₄
11	Glycerol	GLYCEROL	C ₃ H ₈ O ₃
12	Cellulose	CELLULOS	C ₆ H ₁₀ O ₅
13	Zymomonas mobilis	ZM	CO ₂
14	Ash	ASH	C ₆ H ₁₀ O ₅
15	Mesaconic Acid	MESACONIC	C ₅ H ₆ O ₄
16	Fumaric Acid	FUMARIC	C ₄ H ₄ O ₄
17	Aconitic Acid	ACONITIC	C ₆ H ₆ O ₆
18	Glycolic Acid	GLYCOLAC	C ₂ H ₄ O ₃
19	Malic Acid	MALIC	C ₄ H ₆ O ₅
20	Citric Acid	CITRIC	C ₆ H ₈ O ₇
21	Oxalic Acid	OXALIC	C ₂ H ₂ O ₄
22	Carbon Monoxide	CO	CO
23	Hydrogen	H2	H ₂
24	Methane	METHANE	CH ₄
25	Acetaldehyde	ACETALD	C ₂ H ₄ O
26	Hydroxyacetaldehyde	HAA	C ₂ H ₄ O ₂
27	Acetone	ACETONE	C ₃ H ₆ O
28	Hydroxyacetone	HA	C ₃ H ₆ O ₂
29	Pyruvaldehyde	PA	C ₃ H ₄ O ₂
30	Furfural	FURFURAL	C ₅ H ₄ O ₂

Table A1 List of components considered in PRO/II simulations, the alias used, and the chemical formula (cont.)

	Component name	Component alias	Chemical Formula
31	2-Furan methanol	FUROH*	C ₅ H ₆ O ₂
32	5-Hydroxymethyl-furfural	HMF	C ₆ H ₆ O ₃
33	Levoglucosan	LG**	C ₆ H ₁₀ O ₅
34	Char	CHAR	C
35	Hexane	HEXANE	C ₆ H ₁₄
36	2,2-Diethoxypropionate-ethyl-ester	C9ester	C ₉ H ₁₈ O ₄
37	2,3-Anhydro-D-mannose (2,3-AM)	MANNOSE	C ₆ H ₈ O ₄
38	Methyl Isobutyl Ketone	MIBK	C ₆ H ₁₂ O
39	Titanium Dioxide	TIO2	TiO ₂

*FUROH refer to components which have the same formula such as 2-Hydroxy-2-cyclopenten-1-one and 1, 3-Butadiene-1-carboxylic acid.

** LG refer to components which have the same formula such as Anhydro-D-mannose (AM) and 1, 6-Anhydro- β -glucofuranose (1,6-AGF)

Appendix B Composition of Molasses

Table B1 Composition of molasses (Teclu *et al.*, 2009)

%Molasses		
Usual range	Indicative average	Components
17-25	20	Water
30-40	35	Sucrose
4-9	7	Glucose
5-12	9	Fructose
1-5	3	Other reducing substances
2-5	4	Other carbohydrates
7-15	12	Ash
2-6	4.5	Nitrogenous compounds
2-8	5	Non-nitrogenous acid
0.1-1	0.4	Wax, sterols and phospholipids

Table B2 Non-nitrogenous acid of sugar cane (Extracted data from Roberts *et al.*, 1954)

	Liters	Mw	API	SG	density(kg/lit)	kg	mass frac.
Syringic	0.4						
Mesaconic	1.8	130.100	-34.082	1.453	1.453	2.61451	0.038
Fumaric	2.3	116.073	-35.670	1.477	1.477	3.39612	0.050
Succinic	3.5	118.089	-31.599	1.416	1.416	4.95741	0.073
Aconitic	4.6	172.180	-37.922	1.512	1.512	6.95569	0.102
Glycolic	5.9	76.052	-27.972	1.367	1.367	8.064	0.118
Malic	7.8	134.089	-25.732	1.338	1.338	10.4351	0.153
Citric	9.1	192.125	-42.588	1.591	1.591	14.4823	0.213
Oxalic	10	90.036	-49.394	1.723	1.723	17.2338	0.253
						68.1389	1.000

Table B3 Molasses composition for simulation

Component	Mw	%wt	liq	%wt liq	solid	%wt solid
H2O	18.0153	20.10	20.10	23.9521		
C12	342.3	35.18	35.18	41.9162		
C6	180.16	19.10	19.10	22.7545		
Cellulose	162.14	4.02			4.02	25
Ash	105.989	12.06			12.06	75
NH3	17.03	4.52	4.52	5.38922		
Mesaconic	130.100	0.19	0.19	0.22976		
Fumaric	116.073	0.25	0.25	0.29845		
Succinic	118.089	0.37	0.37	0.43566		
Aconitic	172.180	0.51	0.51	0.61126		
Glycolic	76.052	0.59	0.59	0.70866		
Malic	134.089	0.77	0.77	0.91703		
Citric	192.125	1.07	1.07	1.2727		
Oxalic	90.036	1.27	1.27	1.5145		
	100.00	83.92	100	16.08	100	

Appendix C Assumption for Simulation and Calculation of Molasses Composition

- Assumption :
 1. Ethanol production rate 100 kg/hr
 2. Reducing substances as monosaccharide (glucose)
 3. Nitrogen compound as an Ammonia
 4. Other carbohydrate as cellulose
 5. Negligible wax, sterols and phospholipids
- Density of molasses 1.4134 kg/lit
- Density of ethanol 0.7893 kg/lit
- Molasses 1 ton can produce Ethanol 250 Lit which is Ethanol 193.325 kg
So, if we produce 100 kg of ethanol Use 506.78 kilograms of molasses.

Note

A sugar is only a reducing sugar if it has an open chain with an aldehyde or a ketone group. Monosaccharides which contain an aldehyde group are known as aldoses, and those with a ketone group are known as ketoses.

Appendix D Chemical Reactions Implemented in PRO/II

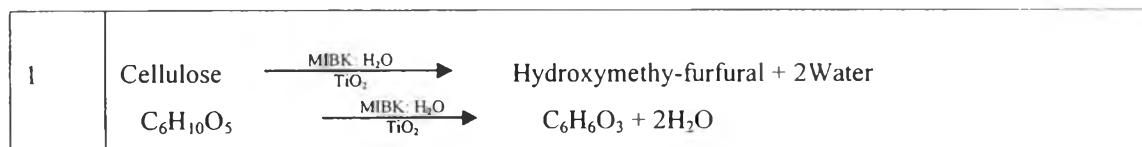
Table D1 List of fermentation reactions that take place in the process and were implemented in PRO/II

1	Cellulose _n + nWater → nGlucose C ₆ H ₁₀ O ₅ + H ₂ O → C ₆ H ₁₂ O ₆
2	Cellulose _n + nWater → nSucrose C ₆ H ₁₀ O ₅ + ½(H ₂ O) → ½C ₁₂ H ₂₂ O ₁₁
3	Sucrose _n + nH ₂ O → 2nGlucose C ₁₂ H ₂₂ O ₁₁ + H ₂ O → 2C ₆ H ₁₂ O ₆
4	Glucose → 2Ethanol + 2Carbon-dioxide C ₆ H ₁₂ O ₆ → 2C ₂ H ₆ O + 2CO ₂
5	Glucose + 1.2Ammonia → 6Z mobilis + 2.4Water + 0.3Oxygen C ₆ H ₁₂ O ₆ + 1.2NH ₃ → 6C _{1.8} H _{0.5} O _{0.2} + 2.4H ₂ O + 0.3O ₂
6	Glucose + 2Water → 2Glycerol + Oxygen C ₆ H ₁₂ O ₆ + 2H ₂ O → 2C ₃ H ₈ O ₃ + O ₂
7	Glucose + 2Carbon-dioxide → 2Succinic-acid + Oxygen C ₆ H ₁₂ O ₆ + 2CO ₂ → 2C ₄ H ₆ O ₄ + O ₂
8	Glucose → 3Acetic-acid C ₆ H ₁₂ O ₆ → 3C ₂ H ₄ O ₂
9	Glucose → 2Lactic-acid C ₆ H ₁₂ O ₆ → 2C ₃ H ₆ O ₃

Table D2 List of decomposition of cellulose reactions that take place in the process and were implemented in PRO/II (Extracted data from Shen and Gu, 2009)

1	Cellulose $C_6H_{10}O_5$	\longrightarrow Hydroxyacetone + 3Carbon Monoxide + 2Hydrogen $C_3H_6O_2 + 3CO + 2H_2$
2	2Cellulose $2C_6H_{10}O_5$	\longrightarrow Hydroxyacetaldehyde + 2 Methane + 4Carbon Monoxide $C_2H_4O_2 + 2CH_4 + 4CO$
3	2Cellulose $2C_6H_{10}O_5$	\longrightarrow Acetone + 9Carbon Monoxide + 7Hydrogen $C_3H_6O_2 + 3CO + 2H_2$
4	Cellulose $C_6H_{10}O_5$	\longrightarrow Hydroxymethyl-furfural + 2Water $C_6H_6O_3 + 2H_2O$
5	5Cellulose $5C_6H_{10}O_5$	\longrightarrow 6Furfural + 13Water $6C_5H_4O_2 + 13H_2O$
6	3Cellulose $3C_6H_{10}O_5$	\longrightarrow Furfural + 13Carbon Monoxide + 13Hydrogen $C_5H_4O_2 + 13CO + 13H_2$
7	Cellulose $C_6H_{10}O_5$	\longrightarrow Furan methanol + 2Water + Carbon Monoxide $C_5H_6O_2 + 2H_2O + CO$
8	3Cellulose $3C_6H_{10}O_5$	\longrightarrow Furan methanol + 13Carbon Monoxide + 12Hydrogen $C_5H_6O_2 + 13CO + 12H_2$
9	2Cellulose $C_6H_{10}O_5$	\longrightarrow Pyruvaldehyde + 2Carbon Monoxide + 3Carbon-dioxide + 4Methane $C_3H_4O_2 + 2CO + 3CO_2 + 4CH_4$
10	2Cellulose $2C_6H_{10}O_5$	\longrightarrow 2Acetaldehyde + 3Methane + 2Carbon Monoxide + 3Carbon-dioxide $2C_2H_4O + 3CH_4 + 2CO + 3CO_2$
11	13Cellulose $13C_6H_{10}O_5$	\longrightarrow 6Hexane + 23Water + 42Carbon Monoxide $6C_6H_{14} + 23H_2O + 42CO$
12	Cellulose $C_6H_{10}O_5$	\longrightarrow Anhydro-D-mannose + 13Water $C_6H_8O_4 + H_2O$
13	7Cellulose $C_6H_{10}O_5$	\longrightarrow 3Diethoxypropionate-ethyl-ester + 8Water + 15Carbon Monoxide $3C_9H_{18}O_4 + 8H_2O + 15CO$
14	Cellulose $C_6H_{10}O_5$	\longrightarrow Levoglucosan $C_6H_{10}O_5$
15	2Cellulose $C_6H_{10}O_5$	\longrightarrow 7Char $7C + 5CO_2 + 10H_2$

Table D3 List of synthesis of HMF reaction from cellulose that take place in the process and were implemented in PRO/II (Extracted data from McNeff *et al.*, 2010)



Appendix E Bioethanol Conversion Process Flowsheet Implemented in PRO/II

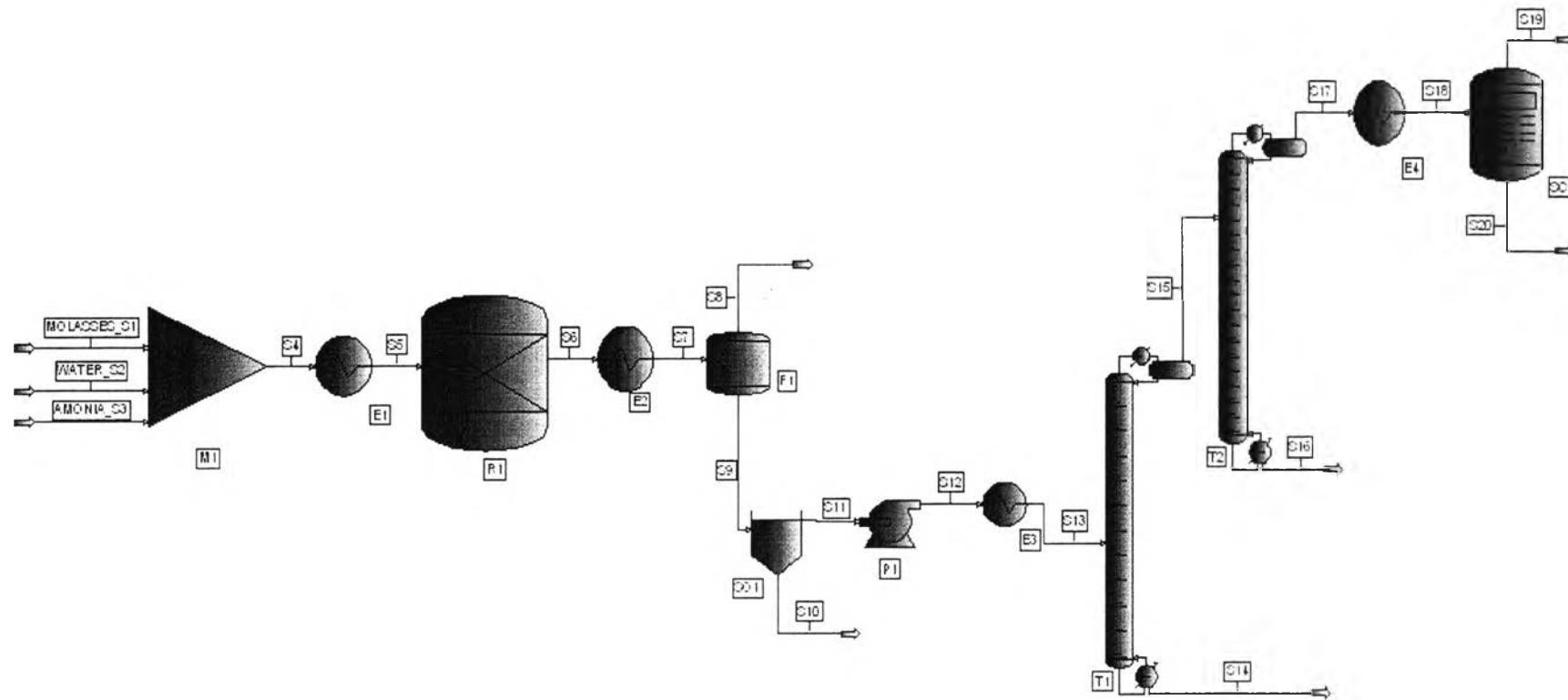


Figure E1 The main operations of the bio-ethanol process from molasses for Base Case Design.

Table E1 Stream summary of the bio-ethanol process from molasses for Base Case Design

Stream Name	MOLASS ES S1	WATER S2	AMONIA S3	S4	S5	S6	S7
Components (kg/h)							
ETHANOL	0.00	0.00	0.00	0.00	0.00	142.37	142.37
WATER	101.86	1400.00	0.00	1501.87	1501.87	1490.81	1490.81
C6	96.77	0.00	0.00	96.77	96.77	22.51	22.51
C12	178.26	0.00	0.00	178.26	178.26	0.00	0.00
ACETACID	0.00	0.00	0.00	0.00	0.00	0.51	0.51
CO2	0.00	0.00	0.00	0.00	0.00	135.91	135.91
O2	0.00	0.00	0.00	0.00	0.00	0.08	0.08
NH3	22.92	0.00	0.01	22.93	22.93	22.86	22.86
LACACID	0.00	0.00	0.00	0.00	0.00	0.30	0.30
SUCCNAC	1.87	0.00	0.00	1.87	1.87	2.12	2.12
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.05	0.05
CELLULOS	20.37	0.00	0.00	20.37	20.37	4.03	4.03
ZM	0.00	0.00	0.00	0.00	0.00	0.54	0.54
ASH	61.12	0.00	0.00	61.12	61.12	61.12	61.12
MESACONIC	0.98	0.00	0.00	0.98	0.98	0.98	0.98
FUMARIC	1.28	0.00	0.00	1.28	1.28	1.28	1.28
ACONITIC	2.59	0.00	0.00	2.59	2.59	2.59	2.59
GLYCOLAC	3.02	0.00	0.00	3.02	3.02	3.02	3.02
MALIC	3.91	0.00	0.00	3.91	3.91	3.91	3.91
CITRIC	5.40	0.00	0.00	5.40	5.40	5.40	5.40
OXALIC	6.42	0.00	0.00	6.42	6.42	6.42	6.42
TotalMass Flow(kg/h)	506.78	1400.00	0.01	1906.79	1906.79	1906.79	1906.79
Temperature (C)	25.00	25.00	25.00	25.00	30.00	30.00	10.00
Pressure (atm)	1.00	1.00	1.00	1.00	1.00	1.00	1.00
EnthalpyFlow (GJ/h)	0.05	0.15	0.00	0.19	0.23	0.23	0.08

Table E1 Stream summary of the bio-ethanol process from molases for Base Case Design (Cont.)

Stream Name	S8	S9	S10	S11	S12	S13	S14
Components (kg/h)							
ETHANOL	0.18	142.19	0.00	142.19	142.19	142.19	0.00
WATER	0.22	1490.59	0.00	1490.59	1490.59	1490.59	894.35
C6	0.00	22.51	0.00	22.51	22.51	22.51	22.51
C12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	0.00	0.51	0.00	0.51	0.51	0.51	0.07
CO2	47.20	88.71	0.00	88.71	88.71	88.71	0.00
O2	0.07	0.01	0.00	0.01	0.01	0.01	0.00
NH3	0.22	22.64	0.00	22.64	22.64	22.64	0.00
LACACID	0.00	0.30	0.00	0.30	0.30	0.30	0.30
SUCCNAC	0.00	2.12	0.00	2.12	2.12	2.12	2.12
GLYCEROL	0.00	0.05	0.00	0.05	0.05	0.05	0.05
CELLULOS	0.00	4.03	4.03	0.00	0.00	0.00	0.00
ZM	0.00	0.54	0.54	0.00	0.00	0.00	0.00
ASH	0.00	61.12	61.12	0.00	0.00	0.00	0.00
MESACONIC	0.00	0.98	0.00	0.98	0.98	0.98	0.98
FUMARIC	0.00	1.28	0.00	1.28	1.28	1.28	1.28
ACONITIC	0.00	2.59	0.00	2.59	2.59	2.59	2.59
GLYCOLAC	0.00	3.02	0.00	3.02	3.02	3.02	3.02
MALIC	0.00	3.91	0.00	3.91	3.91	3.91	3.91
CITRIC	0.00	5.40	0.00	5.40	5.40	5.40	5.40
OXALIC	0.00	6.42	0.00	6.42	6.42	6.42	6.42
Total Mass Flow(kg/h)	47.89	1858.90	65.68	1793.23	1793.23	1793.23	942.99
Temperature (C)	10.00	10.00	10.00	10.00	13.49	116.00	117.07
Pressure (atm)	1.00	1.00	1.00	1.00	2.00	2.00	1.77
Enthalpy Flow (GJ/h)	0.01	0.07	0.00	0.08	0.10	2.23	0.45

Table E1 Stream summary of the bio-ethanol process from molases for Base Case Design (Cont.)

Stream Name	S15	S16	S17	S18	S19	S20
Components (kg/h)						
ETHANOL	142.19	0.00	142.19	142.19	142.19	0.00
WATER	596.24	578.37	17.88	17.88	0.00	17.88
C6	0.00	0.00	0.00	0.00	0.00	0.00
C12	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	0.44	0.41	0.03	0.03	0.00	0.03
CO2	88.71	0.00	88.71	88.71	0.00	88.71
O2	0.01	0.00	0.01	0.01	0.00	0.01
NH3	22.64	0.00	22.64	22.64	0.00	22.64
LACACID	0.00	0.00	0.00	0.00	0.00	0.00
SUCCNAC	0.00	0.00	0.00	0.00	0.00	0.00
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.00
CELLULOS	0.00	0.00	0.00	0.00	0.00	0.00
ZM	0.00	0.00	0.00	0.00	0.00	0.00
ASH	0.00	0.00	0.00	0.00	0.00	0.00
MESACONIC	0.00	0.00	0.00	0.00	0.00	0.00
FUMARIC	0.00	0.00	0.00	0.00	0.00	0.00
ACONITIC	0.00	0.00	0.00	0.00	0.00	0.00
GLYCOLAC	0.00	0.00	0.00	0.00	0.00	0.00
MALIC	0.00	0.00	0.00	0.00	0.00	0.00
CITRIC	0.00	0.00	0.00	0.00	0.00	0.00
OXALIC	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flow(kg/h)	850.23	578.78	271.46	271.46	142.19	129.27
Temperature (C)	111.77	116.85	79.02	141.00	141.00	141.00
Pressure (atm)	1.77	1.77	1.77	1.77	1.77	1.77
Enthalpy Flow (GJ/h)	1.82	0.28	0.24	0.26	0.16	0.10

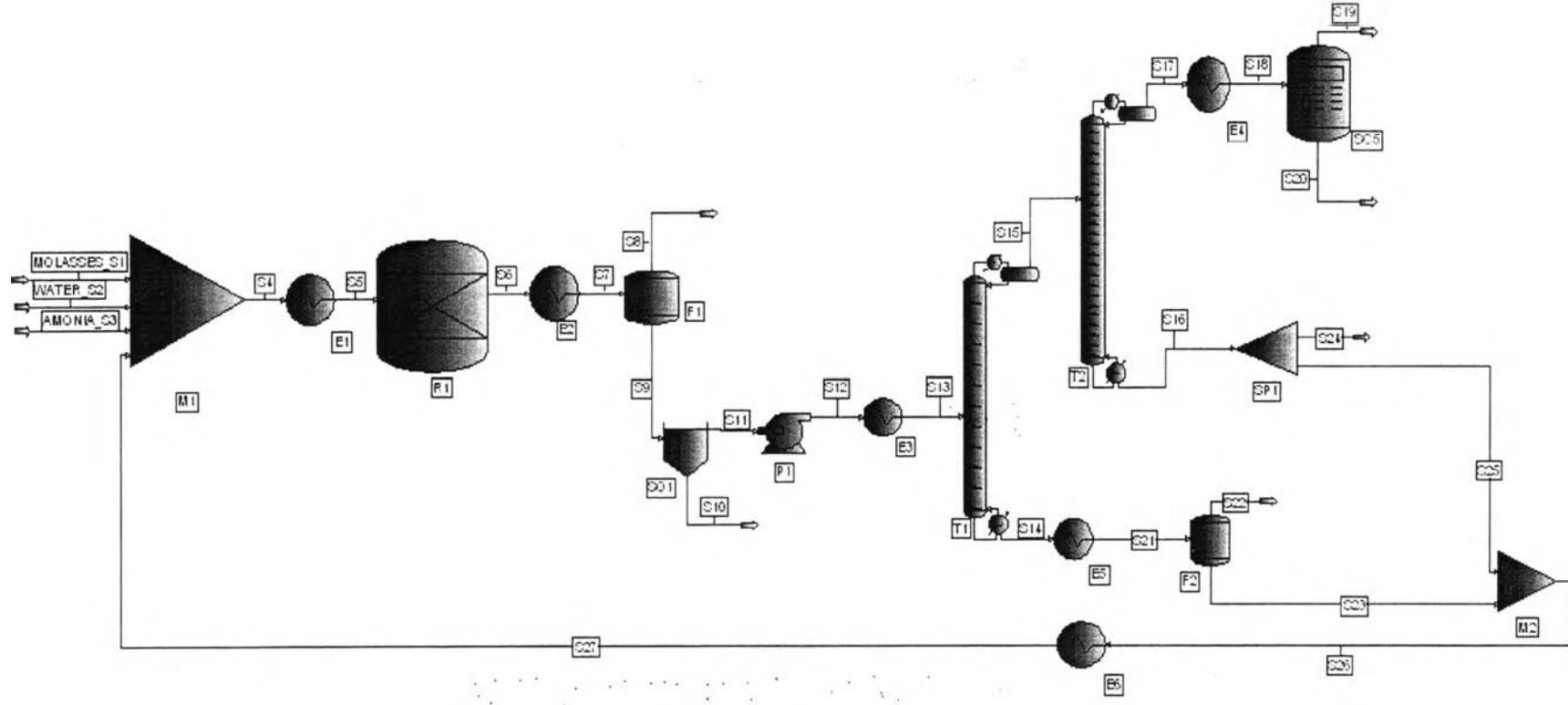


Figure E2 The main operations of the bio-ethanol process from molasses for Alternative 1 (Recycle Glucose and Water).

Table E2 Stream summary of the bio-ethanol process from molasses for Alternative 1 (Recycle Glucose and Water)

Stream Name	MOLASS ES S1	WATER S2	AMONIA S3	S4	S5	S6	S7
Components (kg/h)							
ETHANOL	0.00	0.00	0.00	0.00	0.00	153.75	153.75
WATER	101.86	828.70	0.00	1474.08	1474.08	1463.04	1463.04
C6	96.77	0.00	0.00	120.95	120.95	24.31	24.31
C12	178.26	0.00	0.00	178.26	178.26	0.00	0.00
ACETACID	0.00	0.00	0.00	2.40	2.40	2.96	2.96
CO2	0.00	0.00	0.00	0.00	0.00	146.77	146.77
O2	0.00	0.00	0.00	0.00	0.00	0.08	0.08
NH3	22.92	0.00	0.01	22.93	22.93	22.85	22.85
LACACID	0.00	0.00	0.00	0.00	0.00	0.32	0.32
SUCCNAC	1.87	0.00	0.00	1.88	1.88	2.15	2.15
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.05	0.05
CELLULOS	20.37	0.00	0.00	20.37	20.37	4.03	4.03
ZM	0.00	0.00	0.00	0.00	0.00	0.58	0.58
ASH	61.12	0.00	0.00	61.12	61.12	61.12	61.12
MESACONIC	0.98	0.00	0.00	0.98	0.98	0.98	0.98
FUMARIC	1.28	0.00	0.00	1.28	1.28	1.28	1.28
ACONITIC	2.59	0.00	0.00	2.69	2.69	2.69	2.69
GLYCOLAC	3.02	0.00	0.00	3.02	3.02	3.02	3.02
MALIC	3.91	0.00	0.00	3.94	3.94	3.94	3.94
CITRIC	5.40	0.00	0.00	5.65	5.65	5.65	5.65
OXALIC	6.42	0.00	0.00	6.44	6.44	6.44	6.44
Total Mass Flow(kg/h)	506.78	828.70	0.01	1906.00	1906.00	1906.00	1906.00
Temperature (C)	25.00	25.00	25.00	25.00	30.00	30.00	10.00
Pressure (atm)	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Enthalpy Flow (GJ/h)	0.05	0.09	0.00	0.20	0.23	0.23	0.09

Table E2 Stream summary of the bio-ethanol process from molases for Alternative 1 (Recycle Glucose and Water) (Cont.)

Stream Name	S8	S9	S10	S11	S12	S13	S14
Components (kg/h)							
ETHANOL	0.24	153.51	0.00	153.51	153.51	153.51	0.00
WATER	0.28	1462.76	0.00	1462.76	1462.76	1462.76	877.66
C6	0.00	24.31	0.00	24.31	24.31	24.31	24.31
C12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	0.00	2.95	0.00	2.95	2.95	2.95	0.41
CO2	58.82	87.96	0.00	87.96	87.96	87.96	0.00
O2	0.08	0.01	0.00	0.01	0.01	0.01	0.00
NH3	0.27	22.58	0.00	22.58	22.58	22.58	0.00
LACACID	0.00	0.32	0.00	0.32	0.32	0.32	0.32
SUCCNAC	0.00	2.15	0.00	2.15	2.15	2.15	2.15
GLYCEROL	0.00	0.05	0.00	0.05	0.05	0.05	0.05
CELLULOS	0.00	4.03	4.03	0.00	0.00	0.00	0.00
ZM	0.00	0.58	0.58	0.00	0.00	0.00	0.00
ASH	0.00	61.12	61.12	0.00	0.00	0.00	0.00
MESACONIC	0.00	0.98	0.00	0.98	0.98	0.98	0.98
FUMARIC	0.00	1.28	0.00	1.28	1.28	1.28	1.28
ACONITIC	0.00	2.69	0.00	2.69	2.69	2.69	2.69
GLYCOLAC	0.00	3.02	0.00	3.02	3.02	3.02	3.02
MALIC	0.00	3.94	0.00	3.94	3.94	3.94	3.94
CITRIC	0.00	5.65	0.00	5.65	5.65	5.65	5.65
OXALIC	0.00	6.44	0.00	6.44	6.44	6.44	6.44
Total Mass Flow(kg/h)	59.68	1846.32	65.72	1780.60	1780.60	1780.60	928.90
Temperature (C)	10.00	10.00	10.00	10.00	13.51	116.00	117.08
Pressure (atm)	1.00	1.00	1.00	1.00	2.00	2.00	1.77
Enthalpy Flow (GJ/h)	0.01	0.07	0.00	0.08	0.10	2.28	0.45

Table E2 Stream summary of the bio-ethanol process from molases for Alternative 1 (Recycle Glucose and Water) (Cont.)

Stream Name	S15	S16	S17	S18	S19	S20	S21
Components (kg/h)							
ETHANOL	153.51	0.00	153.51	153.51	153.51	0.00	0.00
WATER	585.10	567.55	17.55	17.55	0.00	17.55	877.66
C6	0.00	0.00	0.00	0.00	0.00	0.00	24.31
C12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	2.54	2.51	0.03	0.03	0.00	0.03	0.41
CO2	87.96	0.00	87.96	87.96	0.00	87.96	0.00
O2	0.01	0.00	0.01	0.01	0.00	0.01	0.00
NH3	22.58	0.00	22.58	22.58	0.00	22.58	0.00
LACACID	0.00	0.00	0.00	0.00	0.00	0.00	0.32
SUCCNAC	0.00	0.00	0.00	0.00	0.00	0.00	2.15
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.00	0.05
CELLULOS	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ZM	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ASH	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MESACONIC	0.00	0.00	0.00	0.00	0.00	0.00	0.98
FUMARIC	0.00	0.00	0.00	0.00	0.00	0.00	1.28
ACONITIC	0.00	0.00	0.00	0.00	0.00	0.00	2.69
GLYCOLAC	0.00	0.00	0.00	0.00	0.00	0.00	3.02
MALIC	0.00	0.00	0.00	0.00	0.00	0.00	3.94
CITRIC	0.00	0.00	0.00	0.00	0.00	0.00	5.65
OXALIC	0.00	0.00	0.00	0.00	0.00	0.00	6.44
Total Mass Flow(kg/h)	851.70	570.07	281.63	281.63	153.51	128.12	928.90
Temperature (C)	111.53	116.84	79.43	141.00	141.00	141.00	320.00
Pressure (atm)	1.77	1.77	1.77	1.77	1.77	1.77	1.77
Enthalpy Flow (GJ/h)	1.80	0.28	0.25	0.27	0.17	0.10	2.39

Table E2 Stream summary of the bio-ethanol process from molases for Alternative 1 (Recycle Glucose and Water) (Cont.)

Stream Name	S22	S23	S24	S25	S26	S27
Components (kg/h)						
ETHANOL	0.00	0.00	0.00	0.00	0.00	0.00
WATER	877.62	0.04	25.11	542.44	542.48	542.48
C6	0.12	24.18	0.00	0.00	24.18	24.18
C12	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	0.41	0.00	0.11	2.40	2.40	2.40
CO2	0.00	0.00	0.00	0.00	0.00	0.00
O2	0.00	0.00	0.00	0.00	0.00	0.00
NH3	0.00	0.00	0.00	0.00	0.00	0.00
LACACID	0.32	0.00	0.00	0.00	0.00	0.00
SUCCNAC	2.14	0.01	0.00	0.00	0.01	0.01
GLYCEROL	0.05	0.00	0.00	0.00	0.00	0.00
CELLULOS	0.00	0.00	0.00	0.00	0.00	0.00
ZM	0.00	0.00	0.00	0.00	0.00	0.00
ASH	0.00	0.00	0.00	0.00	0.00	0.00
MESACONIC	0.98	0.01	0.00	0.00	0.01	0.01
FUMARIC	1.28	0.00	0.00	0.00	0.00	0.00
ACONITIC	2.59	0.10	0.00	0.00	0.10	0.10
GLYCOLAC	3.02	0.00	0.00	0.00	0.00	0.00
MALIC	3.91	0.03	0.00	0.00	0.03	0.03
CITRIC	5.40	0.25	0.00	0.00	0.25	0.25
OXALIC	6.42	0.02	0.00	0.00	0.02	0.02
Total Mass Flow(kg/h)	904.27	24.63	25.22	544.85	569.48	569.48
Temperature (C)	320.00	320.00	116.84	116.84	116.98	25.00
Pressure (atm)	1.77	1.77	1.77	1.77	1.77	1.77
Enthalpy Flow (GJ/h)	2.37	0.02	0.01	0.27	0.28	0.07

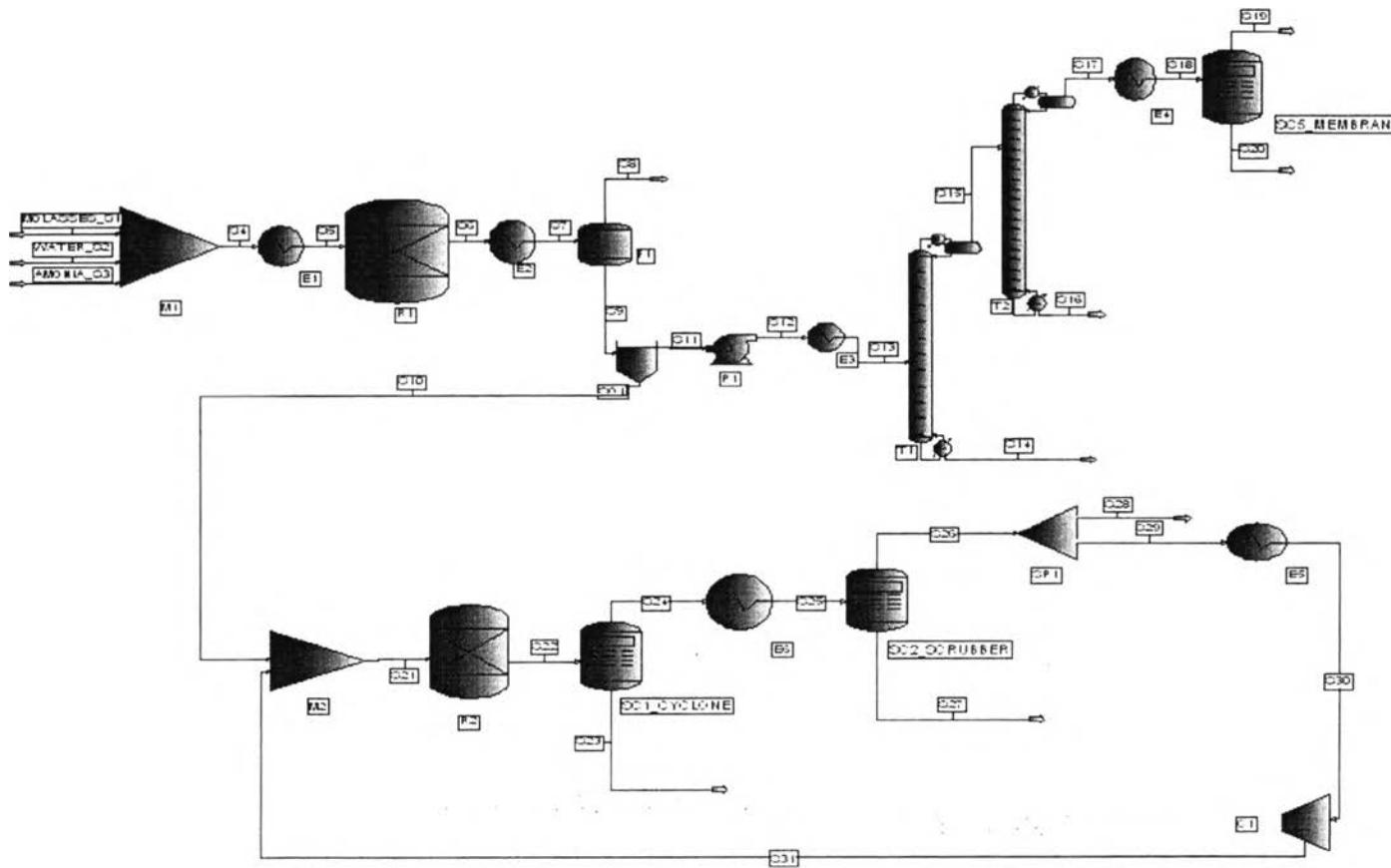


Figure E3 The main operations of the bio-ethanol process from molasses for Alternative 3 (Pyrolysis of Unconverted Cellulose to Produce Biooil).

Table E3 Stream summary of the bio-ethanol process from molasses for Alternative 3 (Pyrolysis of Unconverted Cellulose to Produce Biooil)

Stream Name	MOLASS ES S1	WATER S2	AMONIA S3	S4	S5	S6	S7
Components (kg/h)							
ETHANOL	0.00	0.00	0.00	0.00	0.00	142.37	142.37
WATER	101.87	1400.00	0.00	1501.87	1501.87	1490.82	1490.82
C6	96.77	0.00	0.00	96.77	96.77	22.51	22.51
C12	178.27	0.00	0.00	178.27	178.27	0.00	0.00
ACETACID	0.00	0.00	0.00	0.00	0.00	0.51	0.51
CO2	0.00	0.00	0.00	0.00	0.00	135.91	135.91
O2	0.00	0.00	0.00	0.00	0.00	0.08	0.08
NH3	22.92	0.00	0.01	22.93	22.93	22.86	22.86
LACACID	0.00	0.00	0.00	0.00	0.00	0.30	0.30
SUCCNAC	1.85	0.00	0.00	1.85	1.85	2.10	2.10
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.05	0.05
CELLULOS	20.37	0.00	0.00	20.37	20.37	4.03	4.03
ZM	0.00	0.00	0.00	0.00	0.00	0.54	0.54
ASH	61.12	0.00	0.00	61.12	61.12	61.12	61.12
CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETALD	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HAA	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETONE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HA	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FURFURAL	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FUROH	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HMF	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LG	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CHAR	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEXANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9ester	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MANNOSE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MESA CONIC	0.98	0.00	0.00	0.98	0.98	0.98	0.98
FUMARIC	1.27	0.00	0.00	1.27	1.27	1.27	1.27
ACONITIC	2.60	0.00	0.00	2.60	2.60	2.60	2.60
GLYCOLAC	3.01	0.00	0.00	3.01	3.01	3.01	3.01
MALIC	3.90	0.00	0.00	3.90	3.90	3.90	3.90
CITRIC	5.41	0.00	0.00	5.41	5.41	5.41	5.41
OXALIC	6.44	0.00	0.00	6.44	6.44	6.44	6.44
Total Mass Flow(kg/h)	506.78	1400.00	0.01	1906.79	1906.79	1906.79	1906.79
Temperature (C)	25.00	25.00	25.00	25.00	30.00	30.00	10.00
Pressure (atm)	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Enthalpy Flow (GJ/h)	0.05	0.15	0.00	0.19	0.23	0.23	0.08

Table E3 Stream summary of the bio-ethanol process from molases for Alternative 3 (Pyrolysis of Unconverted Cellulose to Produce Biooil) (Cont.)

Stream Name	S8	S9	S10	S11	S12	S13	S14
Components (kg/h)							
ETHANOL	0.18	142.19	0.00	142.19	142.19	142.19	0.00
WATER	0.22	1490.59	0.00	1490.59	1490.59	1490.59	894.36
C6	0.00	22.51	0.00	22.51	22.51	22.51	22.51
C12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	0.00	0.51	0.00	0.51	0.51	0.51	0.07
CO2	47.20	88.71	0.00	88.71	88.71	88.71	0.00
O2	0.07	0.01	0.00	0.01	0.01	0.01	0.00
NH3	0.22	22.64	0.00	22.64	22.64	22.64	0.00
LACACID	0.00	0.30	0.00	0.30	0.30	0.30	0.30
SUCCNAC	0.00	2.10	0.00	2.10	2.10	2.10	2.10
GLYCEROL	0.00	0.05	0.00	0.05	0.05	0.05	0.05
CELLULOS	0.00	4.03	4.03	0.00	0.00	0.00	0.00
ZM	0.00	0.54	0.54	0.00	0.00	0.00	0.00
ASH	0.00	61.12	61.12	0.00	0.00	0.00	0.00
CO	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
METHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETALD	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HAA	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETONE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HA	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FURFURAL	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FUROH	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HMF	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LG	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CHAR	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEXANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9ester	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MANNOSE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MESACONIC	0.00	0.98	0.00	0.98	0.98	0.98	0.98
FUMARIC	0.00	1.27	0.00	1.27	1.27	1.27	1.27
ACONITIC	0.00	2.60	0.00	2.60	2.60	2.60	2.60
GLYCOLAC	0.00	3.01	0.00	3.01	3.01	3.01	3.01
MALIC	0.00	3.90	0.00	3.90	3.90	3.90	3.90
CITRIC	0.00	5.41	0.00	5.41	5.41	5.41	5.41
OXALIC	0.00	6.44	0.00	6.44	6.44	6.44	6.44
Total Mass Flow(kg/h)	47.89	1858.90	65.68	1793.22	1793.22	1793.22	942.99
Temperature (C)	10.00	10.00	10.00	10.00	13.49	116.00	117.07
Pressure (atm)	1.00	1.00	1.00	1.00	2.00	2.00	1.77
Enthalpy Flow (GJ/h)	0.01	0.07	0.00	0.08	0.10	2.23	0.45

Table E3 Stream summary of the bio-ethanol process from molases for Alternative 3 (Pyrolysis of Unconverted Cellulose to Produce Biooil) (Cont.)

Stream Name	S15	S16	S17	S18	S19	S20	S21
Components (kg/h)							
ETHANOL	142.19	0.00	142.19	142.19	142.19	0.00	0.00
WATER	596.24	578.35	17.89	17.89	0.00	17.89	0.00
C6	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	0.44	0.44	0.00	0.00	0.00	0.00	0.00
CO2	88.71	0.00	88.71	88.71	0.00	88.71	14.22
O2	0.01	0.00	0.01	0.01	0.00	0.01	0.00
NH3	22.64	0.00	22.64	22.64	0.00	22.64	0.00
LACACID	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SUCCNAC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CELLULOS	0.00	0.00	0.00	0.00	0.00	0.00	4.03
ZM	0.00	0.00	0.00	0.00	0.00	0.00	0.54
ASH	0.00	0.00	0.00	0.00	0.00	0.00	61.12
CO	0.00	0.00	0.00	0.00	0.00	0.00	12.44
H2	0.00	0.00	0.00	0.00	0.00	0.00	1.83
METHANE	0.00	0.00	0.00	0.00	0.00	0.00	0.59
ACETALD	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HAA	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETONE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HA	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PA	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FURFURAL	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FUROH	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HMF	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LG	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CHAR	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HEXANE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C9ester	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MANNOSE	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MESACONIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FUMARIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACONITIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GLYCOLAC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MALIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CITRIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OXALIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flow(kg/h)	850.23	578.79	271.44	271.44	142.19	129.25	94.76
Temperature (C)	111.77	116.85	79.01	141.00	141.00	141.00	504.77
Pressure (atm)	1.77	1.77	1.77	1.77	1.77	1.77	1.00
Enthalpy Flow (GJ/h)	1.82	0.28	0.24	0.26	0.16	0.10	0.08

Table E3 Stream summary of the bio-ethanol process from molasses for Alternative 3 (Pyrolysis of Unconverted Cellulose to Produce Biooil) (Cont.)

Stream Name	S22	S23	S24	S25	S26	S27	S28
Components (kg/h)							
ETHANOL	0.00	0.00	0.00	0.00	0.00	0.000	0.00
WATER	0.04	0.00	0.04	0.04	0.00	0.043	0.00
C6	0.00	0.00	0.00	0.00	0.00	0.000	0.00
C12	0.00	0.00	0.00	0.00	0.00	0.000	0.00
ACETACID	0.00	0.00	0.00	0.00	0.00	0.000	0.00
CO2	14.70	0.00	14.70	14.70	14.70	0.000	0.48
O2	0.00	0.00	0.00	0.00	0.00	0.000	0.00
NH3	0.00	0.00	0.00	0.00	0.00	0.000	0.00
LACACID	0.00	0.00	0.00	0.00	0.00	0.000	0.00
SUCCNAC	0.00	0.00	0.00	0.00	0.00	0.000	0.00
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.000	0.00
CELLULOS	0.00	0.00	0.00	0.00	0.00	0.000	0.00
ZM	0.54	0.54	0.00	0.00	0.00	0.000	0.00
ASH	61.12	61.12	0.00	0.00	0.00	0.000	0.00
CO	12.86	0.00	12.86	12.86	12.86	0.000	0.42
H2	1.90	0.00	1.90	1.90	1.90	0.000	0.06
METHANE	0.61	0.00	0.61	0.61	0.61	0.000	0.02
ACETALD	0.00	0.00	0.00	0.00	0.00	0.002	0.00
HAA	0.09	0.00	0.09	0.09	0.00	0.089	0.00
ACETONE	0.04	0.00	0.04	0.04	0.00	0.039	0.00
HA	0.05	0.00	0.05	0.05	0.00	0.052	0.00
PA	0.00	0.00	0.00	0.00	0.00	0.004	0.00
FURFURAL	0.02	0.00	0.02	0.02	0.00	0.023	0.00
FUROH	0.03	0.00	0.03	0.03	0.00	0.029	0.00
HMF	0.07	0.00	0.07	0.07	0.00	0.066	0.00
LG	3.32	0.00	3.32	3.32	0.00	3.317	0.00
CHAR	0.18	0.18	0.00	0.00	0.00	0.000	0.00
HEXANE	0.00	0.00	0.00	0.00	0.00	0.004	0.00
C9ester	0.03	0.00	0.03	0.03	0.00	0.034	0.00
MANNOSE	0.02	0.00	0.02	0.02	0.00	0.020	0.00
MESACONIC	0.00	0.00	0.00	0.00	0.00	0.000	0.00
FUMARIC	0.00	0.00	0.00	0.00	0.00	0.000	0.00
ACONITIC	0.00	0.00	0.00	0.00	0.00	0.000	0.00
GLYCOLAC	0.00	0.00	0.00	0.00	0.00	0.000	0.00
MALIC	0.00	0.00	0.00	0.00	0.00	0.000	0.00
CITRIC	0.00	0.00	0.00	0.00	0.00	0.000	0.00
OXALIC	0.00	0.00	0.00	0.00	0.00	0.000	0.00
Total Mass Flow(kg/h)	95.63	61.84	33.80	33.80	30.08	3.722	0.99
Temperature (C)	500.00	500.00	500.00	22.00	47.39	47.391	47.39
Pressure (atm)	1.00	1.00	1.00	1.00	1.00	1.000	1.00
Enthalpy Flow (GJ/h)	0.29	0.26	0.04	0.00	0.00	-0.006	0.00

Table E3 Stream summary of the bio-ethanol process from molasses for Alternative 3 (Pyrolysis of Unconverted Cellulose to Produce Biooil) (Cont.)

Stream Name	S29	S30	S31
Components (kg/h)			
ETHANOL	0.00	0.00	0.00
WATER	0.00	0.00	0.00
C6	0.00	0.00	0.00
C12	0.00	0.00	0.00
ACETACID	0.00	0.00	0.00
CO2	14.22	14.22	14.22
O2	0.00	0.00	0.00
NH3	0.00	0.00	0.00
LACACID	0.00	0.00	0.00
SUCCNAC	0.00	0.00	0.00
GLYCEROL	0.00	0.00	0.00
CELLULOS	0.00	0.00	0.00
ZM	0.00	0.00	0.00
ASH	0.00	0.00	0.00
CO	12.44	12.44	12.44
H2	1.83	1.83	1.83
METHANE	0.59	0.59	0.59
ACETALD	0.00	0.00	0.00
HAA	0.00	0.00	0.00
ACETONE	0.00	0.00	0.00
HA	0.00	0.00	0.00
PA	0.00	0.00	0.00
FURFURAL	0.00	0.00	0.00
FUROH	0.00	0.00	0.00
HMF	0.00	0.00	0.00
LG	0.00	0.00	0.00
CHAR	0.00	0.00	0.00
HEXANE	0.00	0.00	0.00
C9ester	0.00	0.00	0.00
MANNOSE	0.00	0.00	0.00
MESACONIC	0.00	0.00	0.00
FUMARIC	0.00	0.00	0.00
ACONITIC	0.00	0.00	0.00
GLYCOLAC	0.00	0.00	0.00
MALIC	0.00	0.00	0.00
CITRIC	0.00	0.00	0.00
OXALIC	0.00	0.00	0.00
Total Mass			
Flow(kg/h)	29.08	29.08	29.08
Temperature (C)	47.39	850.00	1160.89
Pressure (atm)	1.00	1.00	3.06
Enthalpy Flow (GJ/h)	0.00	0.06	0.09

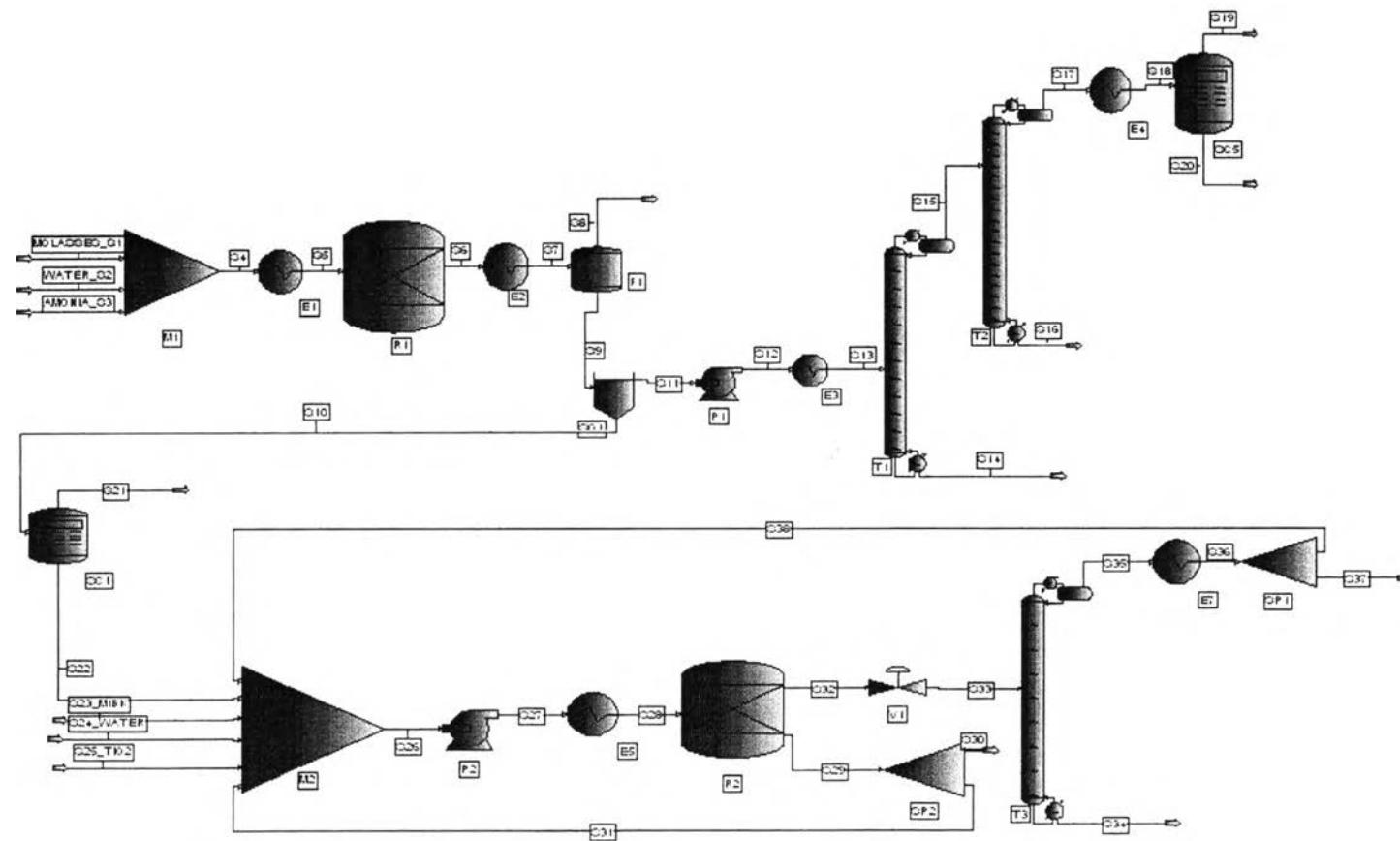


Figure E4 The main operations of the bio-ethanol process from molases for alternative 4 (Production of Hydroxymethyl Furfural from Unconverted Cellulose).

Table E4 Stream summary of the bio-ethanol process from molasses for Alternative 4 (Production of Hydroxymethyl Furfural from Unconverted Cellulose)

Stream Name	MOLASS ES S1	WATER S2	AMONIA S3	S4	S5	S6	S7
Components (kg/h)							
ETHANOL	0.00	0.00	0.00	0.00	0.00	142.16	142.16
WATER	101.78	1398.81	0.00	1500.59	1500.59	1489.55	1489.55
C6	96.69	0.00	0.00	96.69	96.69	22.49	22.49
C12	178.11	0.00	0.00	178.11	178.11	0.00	0.00
ACETACID	0.00	0.00	0.00	0.00	0.00	0.51	0.51
CO2	0.00	0.00	0.00	0.00	0.00	135.88	135.88
O2	0.00	0.00	0.00	0.00	0.00	0.08	0.08
NH3	22.88	0.00	0.01	22.89	22.89	22.82	22.82
LACACID	0.00	0.00	0.00	0.00	0.00	0.30	0.30
SUCCNAC	1.85	0.00	0.00	1.85	1.85	2.10	2.10
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.05	0.05
CELLULOS	20.35	0.00	0.00	20.35	20.35	4.02	4.02
ZM	0.00	0.00	0.00	0.00	0.00	0.54	0.54
ASH	61.12	0.00	0.00	61.12	61.12	61.12	61.12
MIBK	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TIO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HMF	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MESACONIC	0.98	0.00	0.00	0.98	0.98	0.98	0.98
FUMARIC	1.27	0.00	0.00	1.27	1.27	1.27	1.27
ACONITIC	2.60	0.00	0.00	2.60	2.60	2.60	2.60
GLYCOLAC	3.01	0.00	0.00	3.01	3.01	3.01	3.01
MALIC	3.90	0.00	0.00	3.90	3.90	3.90	3.90
CITRIC	5.41	0.00	0.00	5.41	5.41	5.41	5.41
OXALIC	6.44	0.00	0.00	6.44	6.44	6.44	6.44
Total Mass Flow(kg/h)	506.39	1398.81	0.01	1905.21	1905.21	1905.21	1905.21
Temperature (C)	25.00	25.00	25.00	25.00	30.00	30.00	10.00
Pressure (atm)	1.00	1.00	1.00	1.00	1.00	1.00	1.00
Enthalpy Flow (GJ/h)	0.05	0.15	0.00	0.19	0.23	0.23	0.08

Table E4 Stream summary of the bio-ethanol process from molasses for Alternative 4 (Production of Hydroxymethyl Furfural from Unconverted Cellulose) (Cont.)

Stream Name	S8	S9	S10	S11	S12	S13	S14
Components (kg/h)							
ETHANOL	0.18	141.98	0.00	141.98	141.98	141.98	0.00
WATER	0.22	1489.33	0.00	1489.33	1489.33	1489.33	893.60
C6	0.00	22.49	0.00	22.49	22.49	22.49	22.49
C12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	0.00	0.51	0.00	0.51	0.51	0.51	0.07
CO2	47.19	88.69	0.00	88.69	88.69	88.69	0.00
O2	0.07	0.01	0.00	0.01	0.01	0.01	0.00
NH3	0.22	22.60	0.00	22.60	22.60	22.60	0.00
LACACID	0.00	0.30	0.00	0.30	0.30	0.30	0.30
SUCCNAC	0.00	2.10	0.00	2.10	2.10	2.10	2.10
GLYCEROL	0.00	0.05	0.00	0.05	0.05	0.05	0.05
CELLULOS	0.00	4.02	4.02	0.00	0.00	0.00	0.00
ZM	0.00	0.54	0.54	0.00	0.00	0.00	0.00
ASH	0.00	61.12	61.12	0.00	0.00	0.00	0.00
MIBK	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TIO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HMF	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MESACONIC	0.00	0.98	0.00	0.98	0.98	0.98	0.98
FUMARIC	0.00	1.27	0.00	1.27	1.27	1.27	1.27
ACONITIC	0.00	2.60	0.00	2.60	2.60	2.60	2.60
GLYCOLAC	0.00	3.01	0.00	3.01	3.01	3.01	3.01
MALIC	0.00	3.90	0.00	3.90	3.90	3.90	3.90
CITRIC	0.00	5.41	0.00	5.41	5.41	5.41	5.41
OXALIC	0.00	6.44	0.00	6.44	6.44	6.44	6.44
Total Mass Flow(kg/h)	47.88	1857.34	65.67	1791.66	1791.66	1791.66	942.21
Temperature (C)	10.00	10.00	10.00	10.00	13.49	116.00	117.07
Pressure (atm)	1.00	1.00	1.00	1.00	2.00	2.00	1.77
Enthalpy Flow (GJ/h)	0.01	0.07	0.00	0.08	0.10	2.23	0.45

Table E4 Stream summary of the bio-ethanol process from molasses for Alternative 4 (Production of Hydroxymethyl Furfural from Unconverted Cellulose) (Cont.)

Stream Name	S15	S16	S17	S18	S19	S20	S21
Components (kg/h)							
ETHANOL	141.98	0.00	141.98	141.98	141.98	0.00	0.00
WATER	595.73	577.85	17.88	17.88	0.00	17.88	0.00
C6	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	0.44	0.44	0.00	0.00	0.00	0.00	0.00
CO2	88.69	0.00	88.69	88.69	0.00	88.69	0.00
O2	0.01	0.00	0.01	0.01	0.00	0.01	0.00
NH3	22.60	0.00	22.60	22.60	0.00	22.60	0.00
LACACID	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SUCCNAC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CELLULOS	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ZM	0.00	0.00	0.00	0.00	0.00	0.00	0.54
ASH	0.00	0.00	0.00	0.00	0.00	0.00	61.12
MIBK	0.00	0.00	0.00	0.00	0.00	0.00	0.00
TIO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
HMF	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MESACONIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FUMARIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACONITIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GLYCOLAC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MALIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CITRIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OXALIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flow(kg/h)	849.45	578.29	271.16	271.16	141.98	129.18	61.65
Temperature (C)	111.77	116.85	79.01	141.00	141.00	141.00	10.00
Pressure (atm)	1.77	1.77	1.77	1.77	1.77	1.77	1.00
Enthalpy Flow (GJ/h)	1.82	0.28	0.24	0.26	0.16	0.10	0.00

Table E4 Stream summary of the bio-ethanol process from molasses for Alternative 4 (Production of Hydroxymethyl Furfural from Unconverted Cellulose) (Cont.)

Stream Name	S22	S23_MIB K	S24_WA TER	S25_TIO 2	S26	S27	S28
Components (kg/h)							
ETHANOL	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WATER	0.00	0.00	2.70	0.00	47.64	47.64	47.64
C6	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NH3	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LACACID	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SUCCNAC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CELLULOS	4.02	0.00	0.00	0.00	5.01	5.01	5.01
ZM	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ASH	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MIBK	0.00	13.02	0.00	0.00	165.27	165.27	165.27
TIO2	0.00	0.00	0.00	0.80	51.92	51.92	51.92
HMF	0.00	0.00	0.00	0.00	0.05	0.05	0.05
MESACONIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FUMARIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACONITIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GLYCOLAC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MALIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CITRIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OXALIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flow(kg/h)	4.02	13.02	2.70	0.80	269.89	269.89	269.89
Temperature (C)	10.00	25.00	25.00	25.00	42.02	45.66	270.00
Pressure (atm)	1.00	1.00	1.00	1.00	1.00	68.05	68.05
Enthalpy Flow (GJ/h)	-0.01	0.00	0.00	-0.01	-0.50	-0.50	-0.27

Table E4 Stream summary of the bio-ethanol process from molasses for Alternative 4 (Production of Hydroxymethyl Furfural from Unconverted Cellulose) (Cont.)

Stream Name	S29	S30	S31	S32	S33	S34	S35
Components (kg/h)							
ETHANOL	0.00	0.00	0.00	0.00	0.00	0.00	0.00
WATER	0.00	0.00	0.00	48.53	48.53	0.00	48.53
C6	0.00	0.00	0.00	0.00	0.00	0.00	0.00
C12	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACETACID	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CO2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
O2	0.00	0.00	0.00	0.00	0.00	0.00	0.00
NH3	0.00	0.00	0.00	0.00	0.00	0.00	0.00
LACACID	0.00	0.00	0.00	0.00	0.00	0.00	0.00
SUCCNAC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GLYCEROL	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CELLULOS	1.00	0.02	0.99	0.00	0.00	0.00	0.00
ZM	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ASH	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MIBK	0.00	0.00	0.00	165.27	165.27	0.02	165.25
TIO2	51.92	0.80	51.12	0.00	0.00	0.00	0.00
HMF	0.00	0.00	0.00	3.17	3.17	3.11	0.06
MESACONIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
FUMARIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ACONITIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
GLYCOLAC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
MALIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
CITRIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
OXALIC	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Total Mass Flow(kg/h)	52.92	0.81	52.11	216.97	216.97	3.13	213.84
Temperature (C)	270.00	270.00	270.00	270.00	143.70	160.87	90.59
Pressure (atm)	68.05	68.05	68.05	68.05	1.00	1.00	1.00
Enthalpy Flow (GJ/h)	-0.51	-0.01	-0.50	0.24	0.24	0.00	0.22

Table E4 Stream summary of the bio-ethanol process from molasses for Alternative 4 (Production of Hydroxymethyl Furfural from Unconverted Cellulose) (Cont.)

Stream Name	S36	S37	S38
Components (kg/h)			
ETHANOL	0.00	0.00	0.00
WATER	48.53	3.82	44.71
C6	0.00	0.00	0.00
C12	0.00	0.00	0.00
ACETACID	0.00	0.00	0.00
CO2	0.00	0.00	0.00
O2	0.00	0.00	0.00
NH3	0.00	0.00	0.00
LACACID	0.00	0.00	0.00
SUCCNAC	0.00	0.00	0.00
GLYCEROL	0.00	0.00	0.00
CELLULOS	0.00	0.00	0.00
ZM	0.00	0.00	0.00
ASH	0.00	0.00	0.00
MIBK	165.25	13.00	152.24
TIO2	0.00	0.00	0.00
HMF	0.06	0.00	0.06
MESACONIC	0.00	0.00	0.00
FUMARIC	0.00	0.00	0.00
ACONITIC	0.00	0.00	0.00
GLYCOLAC	0.00	0.00	0.00
MALIC	0.00	0.00	0.00
CITRIC	0.00	0.00	0.00
OXALIC	0.00	0.00	0.00
Total Mass Flow(kg/h)	213.84	16.83	197.01
Temperature (C)	25.00	25.00	25.00
Pressure (atm)	1.00	1.00	1.00
Enthalpy Flow (GJ/h)	0.01	0.00	0.01

Appendix F Life Cycle Inventory Analysis of New Design Alternatives

F.1 Alternative-1

Table F1.1 List of inventory of alternative 1 in sugarcane plantation stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Fuel:</i>			<i>Product</i>		
Diesel	1.39E-02	kg	Sugarcane	13.883	kg
<i>Chemical:</i>					
Fertilizer (N)	2.06E-02	kg			
Fertilizer (P)	9.59E-03	kg			
Fertilizer (K)	8.55E-03	kg			
Paraquat (Bipyridylum)	1.49E-04	kg			
Glyphosate	2.38E-05	kg			
Atrazine	5.21E-04	kg			
Ametryne	3.72E-04	kg			
2,4-D	1.49E-04	kg			

Table F1.2 List of inventory of alternative 1 in sugarcane milling stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Raw material:</i>			<i>Product</i>		
Sugarcane plant	13.883	kg	Molasses	3.301	kg
<i>Energy:</i>			<i>Avoid Product</i>		
Production of Electricity & Steam			Electricity	0.406	kWh
Bagasse mainly & other	3.865	kg			
-Electricity from bagasse	0.241	kWh			
-Steam from bagasse	6.242	kg			
<i>Chemical:</i>					
Lime	2.93E-02	kg			
Sodium chloride	1.09E-02	kg			
Hydrochloric acid	6.25E-06	kg			
SiO ₂	3.21E-05	kg			
Biocide	5.09E-05	kg			
Aluminium sulfate	5.18E-05	kg			
Caustic soda flake	1.61E-05	kg			
Flocculants (Iron sulphate)	5.35E-04	kg			
Miscellaneous	7.94E-05	kg			

Table F1.3 List of inventory of alternative 1 in fermentation stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
Material			Product		
Molasses	3.301	Kg	Output-1 From fermentation stage	11.592	Kg
Water	5.398	Kg			
Ammonia	0.000	Kg	Final waste flow		
			Residues	0.428	Kg
Utilities			Emission to Air		
Steam(1 bar)	9.84E-02	Kg	Ethanol	1.56E-03	Kg
			Water	1.81E-03	Kg
			Acetic acid	7.18E-06	Kg
			Carbondioxide	3.84E-01	Kg
			Oxygen	4.90E-04	Kg
			Ammonia	1.77E-03	Kg

Table F1.4 List of inventory of alternative 1 in recovery stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
Material			Product		
Output-1 From fermentation stage	11.592	kg	Ethanol 99.5 wt%	1.000	kg
Energy					
Steam	17.309	kg			
Electricity	0.045	kW	Liquid waste		
			Waste water	6.884	kg

Table F1.5 List of inventory of alternative 1 in biogas and cogeneration stage

F.2 Alternative-2

Table F2.1 List of inventory of alternative 2 in sugarcane plantation stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Fuel:</i>			<i>Product</i>		
Diesel	1.50E-02	kg	Sugarcane	14.988	kg
<i>Chemical:</i>					
Fertilizer (N)	2.22E-02	kg			
Fertilizer (P)	1.04E-02	kg			
Fertilizer (K)	9.23E-03	kg			
Paraquat (Bipyridylum)	1.61E-04	kg			
Glyphosate	2.57E-05	kg			
Atrazine	5.62E-04	kg			
Ametryne	4.01E-04	kg			
2,4-D	1.61E-04	kg			

Table F2.2 List of inventory of alternative 2 in sugarcane milling stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Raw material:</i>			<i>Product</i>		
Sugarcane plant	14.988	kg	Molasses	3.564	kg
			<i>Avoid Product</i>		
<i>Energy:</i>			Electricity	0.438	kWh
Production of Electricity & Steam					
Bagasse mainly & other	4.172	kg			
-Electricity from bagasse	0.260	kWh			
-Steam from bagasse	6.739	kg			
<i>Chemical:</i>					
Lime	3.16E-02	kg			
Sodium chloride	1.18E-02	kg			
Hydrochloric acid	6.74E-06	kg			
SiO ₂	3.47E-05	kg			
Biocide	5.49E-05	kg			
Aluminium sulfate	5.59E-05	kg			
Caustic soda flake	1.73E-05	kg			
Flocculants (Iron sulphate)	5.78E-04	kg			
Miscellaneous	8.57E-05	kg			

Table F2.3 List of inventory of alternative 2 in sugarcane fermentation stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Material</i>			<i>Product</i>		
Molasses	3.564	kg	Output-1 From fermentation stage	12.612	kg
Water	9.846	kg			
Ammonia	7.75E-05	kg			
<i>Utilities</i>			<i>Emission to Air</i>		
Steam	0.106	kg	Ethanol	1.25E-03	kg
			Water	3.85E-01	kg
			Acetic acid	1.08E-06	kg
			Carbondioxide	1.46E+00	kg
			Oxygen	4.78E-04	kg
			Ammonia	1.53E-03	kg
			Nitrogen	4.29E-04	kg

Table F2.4 List of inventory of alternative 2 in sugarcane recovery stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Material</i>			<i>Product</i>		
Output-1	12.612	kg	Ethanol 99.5 wt%	1.000	kg
<i>Energy</i>			<i>Liquid waste</i>		
Steam	8.710	kg	Waste water	11.612	kg
Electricity	0.048	kWh			

Table F2.5 List of inventory of alternative 2 in sugarcane biogas and cogeneration stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Material</i>			<i>Product</i>		
Waste water	11.612	Kg	Cogen Steam	2.325	kg
			Cogen Electricity	0.625	KWh
			<i>Emission to air</i>		
			Nitrogen oxides	1.13E-04	kg
			Carbon monoxide, biogenic	3.60E-04	kg
			Methane, biogenic	1.73E-04	kg
			NM VOC	1.50E-05	kg
			Dinitrogen monoxide	1.88E-05	kg
			Sulfur dioxide	1.58E-04	kg
			Platinum	5.26E-11	kg
			Heat, waste	6.66E+00	MJ
			Used mineral oil, to waste incineration	6.20E-05	kg

F.3 Alternative-3

Table F3.1 List of inventory of alternative 3 in sugarcane plantation stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Fuel:</i>			<i>Product</i>		
Diesel	1.44E-02	kg	Sugarcane	14.418	kg
<i>Chemical:</i>					
Fertilizer (N)	2.14E-02	kg			
Fertilizer (P)	9.96E-03	kg			
Fertilizer (K)	8.88E-03	kg			
Paraquat (Bipyridylium)	1.54E-04	kg			
Glyphosate	2.47E-05	kg			
Atrazine	5.41E-04	kg			
Ametryne	3.86E-04	kg			
2,4-D	1.54E-04	kg			

Table F3.2 List of inventory of alternative 3 in sugarcane milling stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Raw material:</i>			<i>Product</i>		
Sugarcane plant	14.418	kg	Molasses	3.429	kg
<i>Energy:</i>			<i>Avoid Product</i>		
Production of Electricity & Steam			Electricity	0.422	kWh
Bagasse mainly & other	4.014	kg			
-Electricity from bagasse	0.251	kWh			
-Steam from bagasse	6.483	kg			
<i>Chemical:</i>					
Lime	3.04E-02	kg			
Sodium chloride	1.13E-02	kg			
Hydrochloric acid	6.49E-06	kg			
SiO ₂	3.34E-05	kg			
Biocide	5.28E-05	kg			
Aluminium sulfate	5.38E-05	kg			
Caustic soda flake	1.67E-05	kg			
Flocculants (Iron sulphate)	5.56E-04	kg			
Miscellaneous	8.25E-05	kg			

Table F3.3 List of inventory of alternative 3 in sugarcane fermentation stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Material</i>			<i>Product</i>		
Molasses	3.429	kg	Output-1 From fermentation stage	12.133	kg
Water	9.472	kg	Solid stream	0.444	kg
Ammonia	7.46E-05	kg			
<i>Utilities</i>			<i>Emission to Air</i>		
Steam	0.102	kg	Ethanol	1.20E-03	kg
			Water	1.51E-03	kg
			Acetic acid	1.04E-06	kg
			Carbondioxide	3.19E-01	kg
			Oxygen	4.60E-04	kg
			Ammonia	1.47E-03	kg

Table F3.4 List of inventory of alternative 3 in sugarcane recovery stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
Material			Product		
Output-1 From fermentation stage	12.133	Kg	Ethanol 99.5 wt%	1.000	Kg
Energy			Liquid waste		
Steam	10.296	Kg	Waste water	11.612	Kg
Electricity	0.048	kW			

Table F3.5 List of inventory of alternative 3 in sugarcane biogas and cogeneration stage

Table F3.6 List of inventory of alternative 3 in pyrolysis stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Material</i>			<i>Product</i>		
Solid stream	0.444	kg	Bio-oil	0.026	kg
<i>Energy</i>			<i>Emission to air</i>		
Electricity	0.114	kWh	Carbondioxide	1.09E+00	kg
			Water	3.72E-01	kg
			Nitrogen	4.29E-04	kg

F.4 Alternative-4

Table F4.1 List of inventory of alternative 4 in sugarcane plantation stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
<i>Fuel:</i>			<i>Product</i>		
Diesel	1.39E-02	kg	Sugarcane	13.889	kg
<i>Chemical:</i>					
Fertilizer (N)	2.06E-02	kg			
Fertilizer (P)	9.60E-03	kg			
Fertilizer (K)	8.56E-03	kg			
Paraquat (Bipyridylium)	1.49E-04	kg			
Glyphosate	2.38E-05	kg			
Atrazine	5.21E-04	kg			
Ametryne	3.72E-04	kg			
2,4-D	1.49E-04	kg			

Table F4.2 List of inventory of alternative 4 in sugarcane milling stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
Raw material:			Product		
Sugarcane plant	13.889	kg	Molasses	3.303	kg
Energy:			Avoid Product		
Production of Electricity & Steam			Electricity	0.406	kWh
Bagasse mainly & other	3.866	kg			
-Electricity from bagasse	0.241	kWh			
-Steam from bagasse	6.245	kg			
Chemical:					
Lime	2.93E-02	kg			
Sodium chloride	1.09E-02	kg			
Hydrochloric acid	6.25E-06	kg			
SiO ₂	3.21E-05	kg			
Biocide	5.09E-05	kg			
Aluminium sulfate	5.18E-05	kg			
Caustic soda flake	1.61E-05	kg			
Flocculants (Iron sulphate)	5.36E-04	kg			
Miscellaneous	7.95E-05	kg			

Table F4.3 List of inventory of alternative 4 in sugarcane fermentation stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
Material			Product		
Molasses	3.303	kg	Output-1 From fermentation stage	11.687	kg
Water	9.124	kg	Solid stream	0.428	kg
Ammonia	7.18E-05	kg			
			Emission to Air		
Utilities			Ethanol	1.16E-03	kg
Steam(1 bar)	0.098	kg	Water	1.46E-03	kg
			Acetic acid	1.00E-06	kg
			Carbon dioxide	3.08E-01	kg
			Oxygen	4.43E-04	kg
			Ammonia	1.42E-03	kg

Table F4.4 List of inventory of alternative 4 in sugarcane recovery stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
Material			Product		
Output-1 From fermentation stage	11.687	Kg	Ethanol 99.5 wt%	1.000	Kg
Energy			Liquid waste		
Steam	10.296	Kg	Waste water	11.612	Kg
Electricity	0.048	kW			

Table F4.5 List of inventory of alternative 4 in sugarcane biogas and cogeneration stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
Material			Product		
Waste water	11.612	Kg	Steam	2.325	Kg
			Electricity	0.625	KWh
			Emission to air		
			Nitrogen oxides	1.13E-04	kg
			Carbon monoxide, biogenic	3.60E-04	kg
			Methane, biogenic	1.73E-04	kg
			NMVOC	1.50E-05	kg
			Dinitrogen monoxide	1.88E-05	kg
			Sulfur dioxide	1.58E-04	kg
			Platinum	5.26E-11	kg
			Heat, waste	6.66E+00	MJ
			Used mineral oil, to waste incineration	6.20E-05	kg

Table F4.6 List of inventory of alternative 4 in HMF production stage

Input Inventory			Output Inventory		
Type	Amount	Unit	Type	Amount	Unit
Material			Product		
Solid Stream	0.462	kg	HMF	0.022	kg
MIBK	0.092	kg	Final waste flow		
Water	0.019	kg	Residues	0.434	kg
Utilities			Waste and emissions to treatment		
Steam	1.240	kg	Disposal, solvents mixture	0.118	kg
Electricity	0.004	kWh			

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Proceedings:

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