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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

	Compnent name	Component alias	Chemical Formula
1	Ethanol	ETHANOL	C_2H_6O
2	Water	WATER	H_2O
3	Glucose	C6	$C_6H_{12}O_6$
4	Xylose	C5	$C_5H_{10}O_5$
5	Arabinose	C5A	$C_5H_{10}O_5$
6	Mannose	C6M	$C_6H_{12}O_6$
7	Cellobiose	C12	$C_{12}H_{22}O_{11}$
8	Corn Steep Liqior	CLS	H_2O
9	Acetic Acid	ACETACID	$C_2H_4O_2$
10	Sulphuric Acid	SULFURIC	H_2SO_4
11	Furfural	FURFURAL	$C_5H_4O_2$
12	Hydroxymethyl Furfural	HMF	$C_6H_6O_3$
13	Carbondioxide	CO2	CO_2
14	Oxygen	O2	O_2
15	Ammonia	NH3	NH_3
16	Xylitol	XYLITOL	$C_5H_{12}O_5$
17	Lactic Acid	LACACID	$C_3H_6O_3$
18	Succinic Acid	SUCCNAC	$C_4H_6O_4$
19	Glycerol	GLYCEROL	$C_3H_8O_3$
20	Cellulose	CELLULOS	$C_6H_{10}O_5$
21	Hemicellulose	HCELLULO	$C_5H_8O_4$
22	Arabinan	ARABINAN	$C_5H_8O_4$
23	Mannan	MANNAN	$C_6H_{10}O_5$
24	Cellulase (enzyme)	CELLULAC	$CH_{1.57}NOS$
25	Zymomonas Mobilis (bacteria)	ZM	$CH_{1.8}O_{0.5}N_{0.2}$
26	Lignin	LIGNIN	$C_{7.3}H_{13.9}O_{1.3}$
27	Calcium Sulphate	CASO4	$CaSO_4$
28	Calcium Hydroxide	CAHYDROX	$Ca(OH)_2$

Appendix B Chemical Reactions Implemented in PRO/II

Table B1 List of reactions that take place in the process and were implemented in PRO/II

1	Cellulose$_n$ + nWater $\longrightarrow$ nGlucose $C_2H_{10}O_5 + H_2O \longrightarrow C_6H_{12}O_6$
2	Cellulose$_n$ + nWater $\longrightarrow$ nCellobiose $C_6H_{10}O_5 + \frac{1}{2}(H_2O) \longrightarrow \frac{1}{2}C_{12}H_{22}O_{11}$
3	Hemicellulose$_n$ + nWater $\longrightarrow$ nXylose $C_5H_8O_4 + H_2O \longrightarrow C_5H_{10}O_5$
4	Hemicellulose$_n$ $\longrightarrow$ nFurfural + 2nWater $C_5H_8O_4 \longrightarrow C_5H_4O_2 + 2H_2O$
5	Mannan$_n$ + nWater $\longrightarrow$ nMannose $C_6H_{10}O_5 + H_2O \longrightarrow C_6H_{12}O_6$
6	Mannan$_n$ $\longrightarrow$ nHMF + 2nWater $C_6H_{10}O_5 \longrightarrow C_6H_6O_3 + 2H_2O$
7	Arabinan$_n$ + nWater $\longrightarrow$ nArabinose $C_5H_8O_4 + H_2O \longrightarrow C_5H_{10}O_5$
8	Arabinan$_n$ $\longrightarrow$ nFurfural + 2nWater $C_5H_8O_4 \longrightarrow C_5H_4O_2 + 2H_2O$
9	Sulfuric-acid + Calcium-hydroxide $\longrightarrow$ Gypsum $H_2SO_4 + Ca(OH)_2 \longrightarrow CaSO_4{*}2H_2O$
10	3Xylose $\longrightarrow$ 5Ethanol + 5Carbon-dioxide $3C_5H_5O_5 \longrightarrow 5C_2H_6O + 5CO_2$
11	Xylose + Ammonia $\longrightarrow$ 5Z mobilis + 2Water + 0.25Oxygen $C_5H_{10}O_5 + NH_3 \longrightarrow 5C_{1.8}H_{0.5}O_{0.2} + 2H_2O + 0.25O_2$
12	3Xylose + 5Water $\longrightarrow$ 5Glycerol + 2.5Oxygen $3C_5H_{10}O_5 + 5H_2O \longrightarrow 5C_3H_8O_3 + 2.5O_2$
13	Xylose + Water $\longrightarrow$ Xylitol + 0.5Oxygen $C_5H_{10}O_5 + H_2O \longrightarrow C_5H_{12}O_5 + 0.5O_2$
14	3Xylose + 5Carbon-dioxide $\longrightarrow$ 5Succinic-acid + 2.5Oxygen $3C_5H_{10}O_5 + 5CO_2 \longrightarrow 5C_4H_6O_4 + 2.5O_2$
15	2Xylose $\longrightarrow$ 5Acetic-acid $2C_5H_{10}O_5 \longrightarrow 5C_2H_4O_2$
16	3Xylose $\longrightarrow$ 5Lactic-acid $3C_5H_{10}O_5 \longrightarrow 5C_3H_6O_3$
17	3Arabinose $\longrightarrow$ 5Lactic-acid $3C_5H_{10}O_5 \longrightarrow 5C_3H_6O_3$
18	Cellobiose$_n$ + nH_2O $\longrightarrow$ 2nGlucose $C_{12}H_{22}O_{11} + H_2O \longrightarrow 2C_6H_{12}O_6$
19	Glucose $\longrightarrow$ 2Ethanol + 2Carbon-dioxide $C_6H_{12}O_6 \longrightarrow 2C_2H_6O + 2CO_2$
20	Glucose + 1.2Ammonia $\longrightarrow$ 6Z mobilis + 2.4Water + 0.3Oxygen $C_6H_{12}O_6 + 1.2NH_3 \longrightarrow 6C_{1.8}H_{0.5}O_{0.2} + 2.4H_2O + 0.3O_2$
21	Glucose + 2Water $\longrightarrow$ 2Glycerol + Oxygen $C_6H_{12}O_6 + 2H_2O \longrightarrow 2C_3H_8O_3 + O_2$
22	Glucose + 2Carbon-dioxide $\longrightarrow$ 2Succinic-acid + Oxygen $C_6H_{12}O_6 + 2CO_2 \longrightarrow 2C_4H_6O_4 + O_2$
23	Glucose $\longrightarrow$ 3Acetic-acid $C_6H_{12}O_6 \longrightarrow 3C_2H_4O_2$
24	Glucose $\longrightarrow$ 2Lactic-acid $C_6H_{12}O_6 \longrightarrow 2C_3H_6O_3$
25	Mannose $\longrightarrow$ 2Lactic-acid $C_6H_{12}O_6 \longrightarrow 2C_3H_6O_3$

Appendix C Bioethanol Conversion Process Flowsheet Implemented in PRO/II

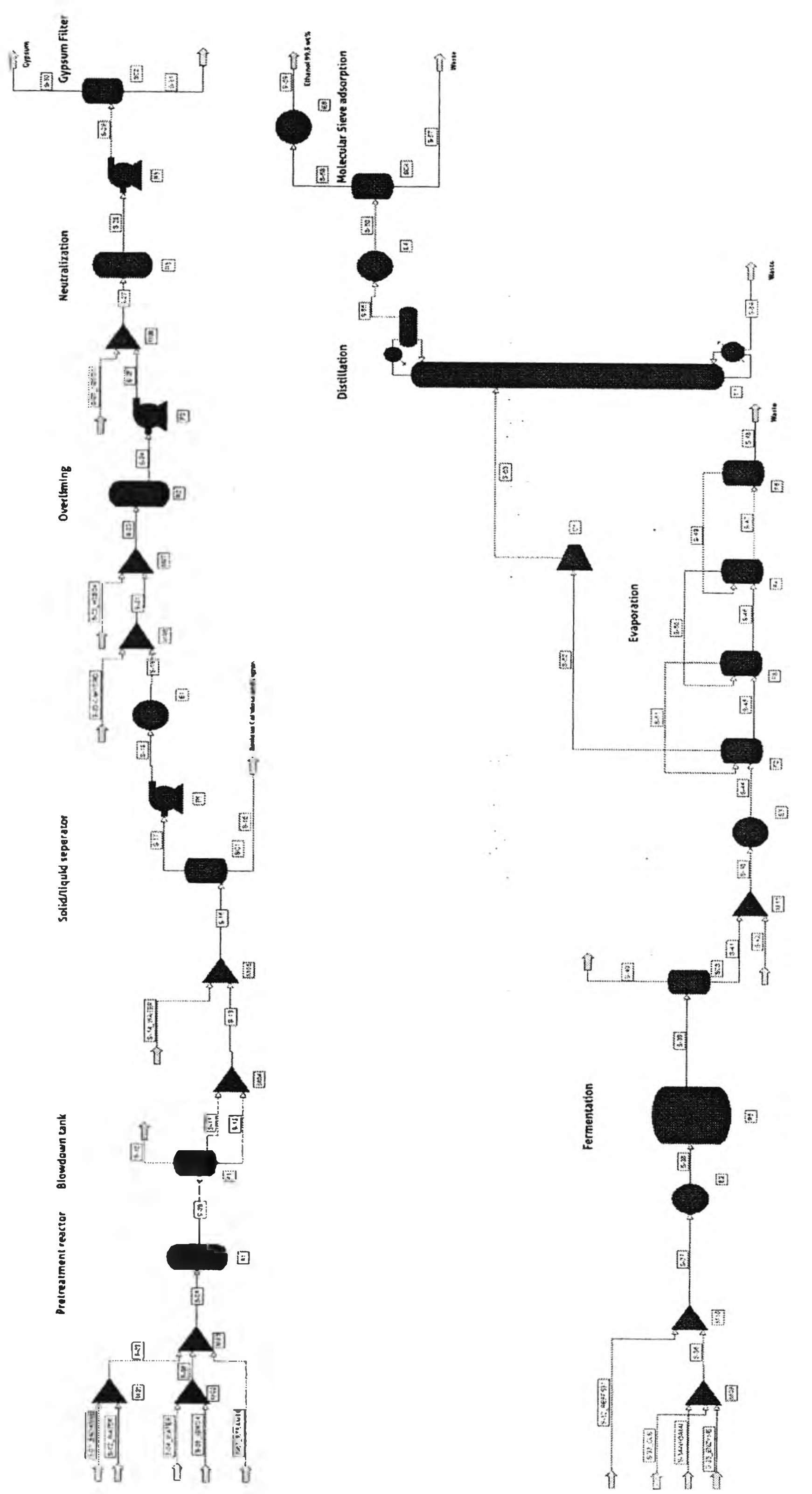

Figure C1 Flowsheet of the TRE design implemented in PRO/II.

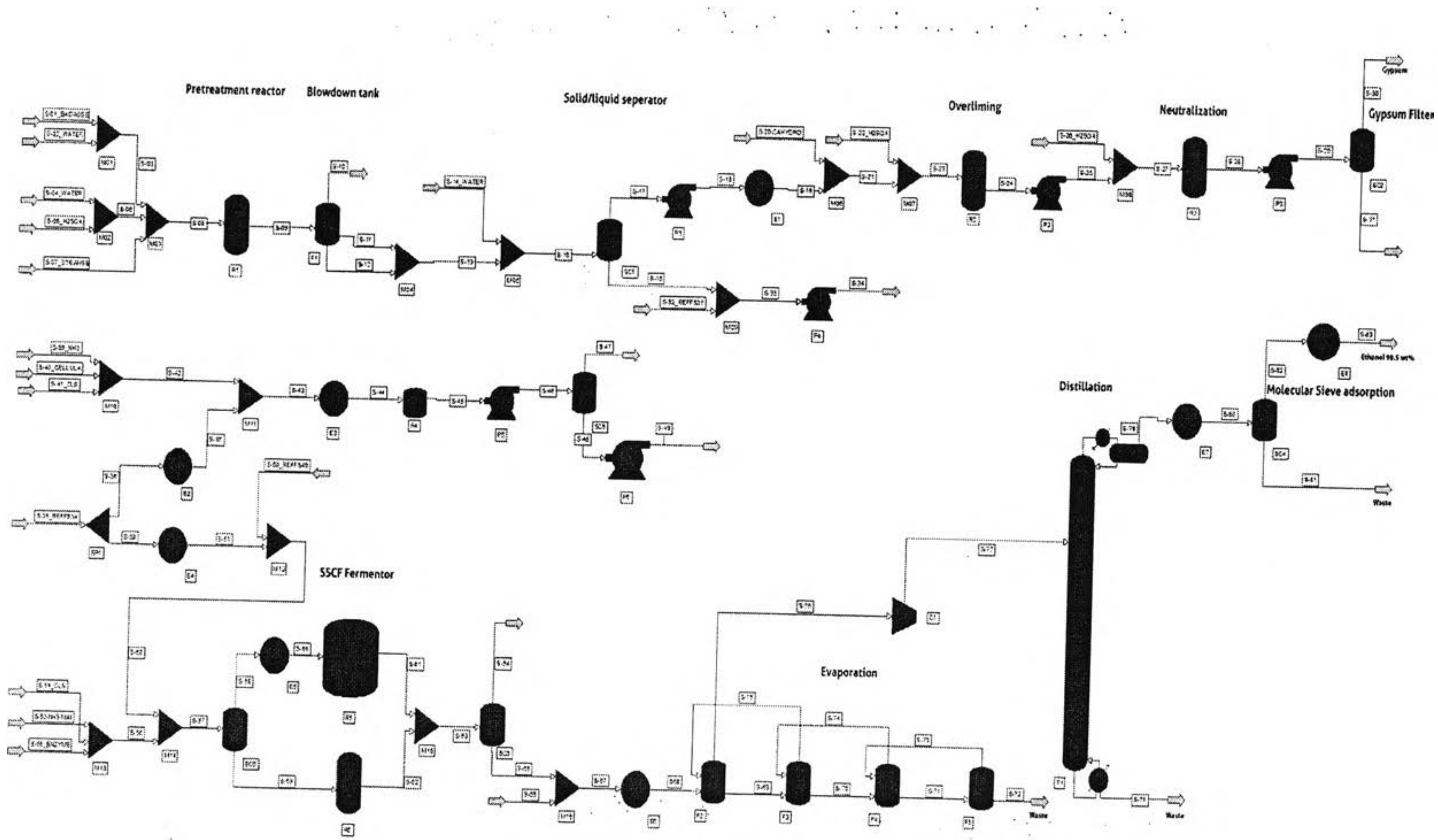

Figure C2 Flowsheet of the base case design and Alternative-1 implemented in PRO/II.

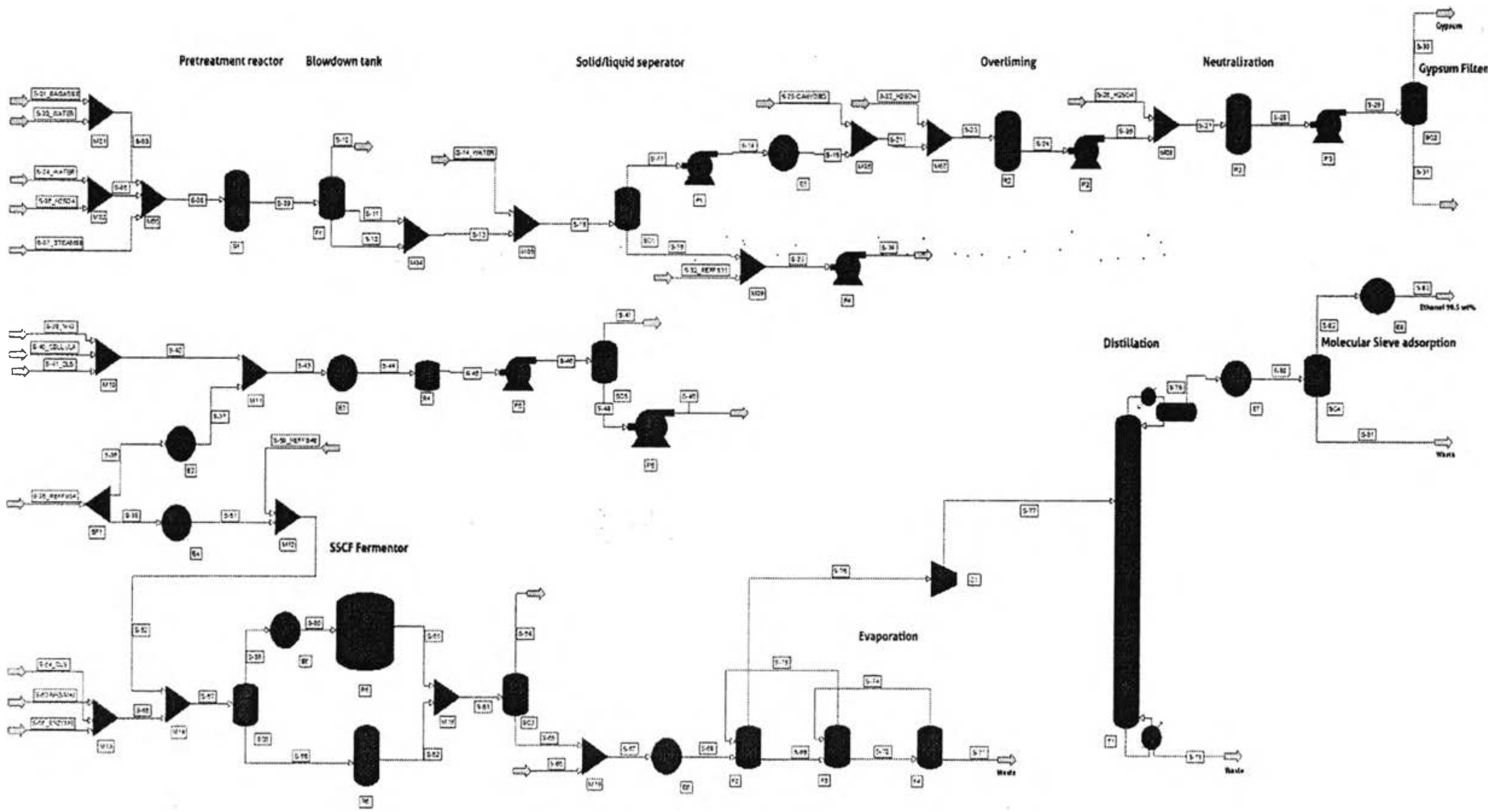

Figure C3 Flowsheet of the Alternative-2 implemented in PRO/II.

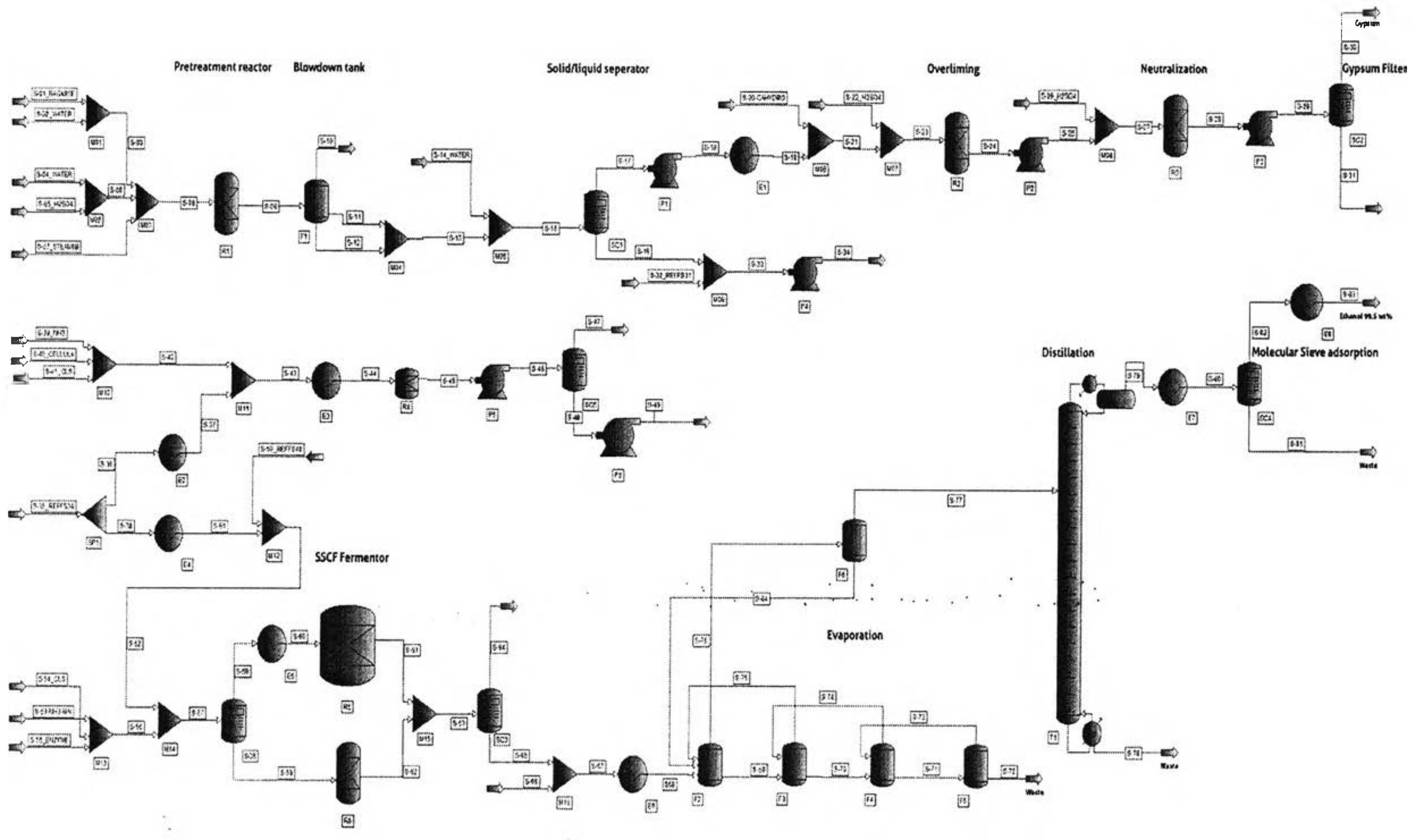

Figure C4 Flowsheet of the Alternative-3 implemented in PRO/II.

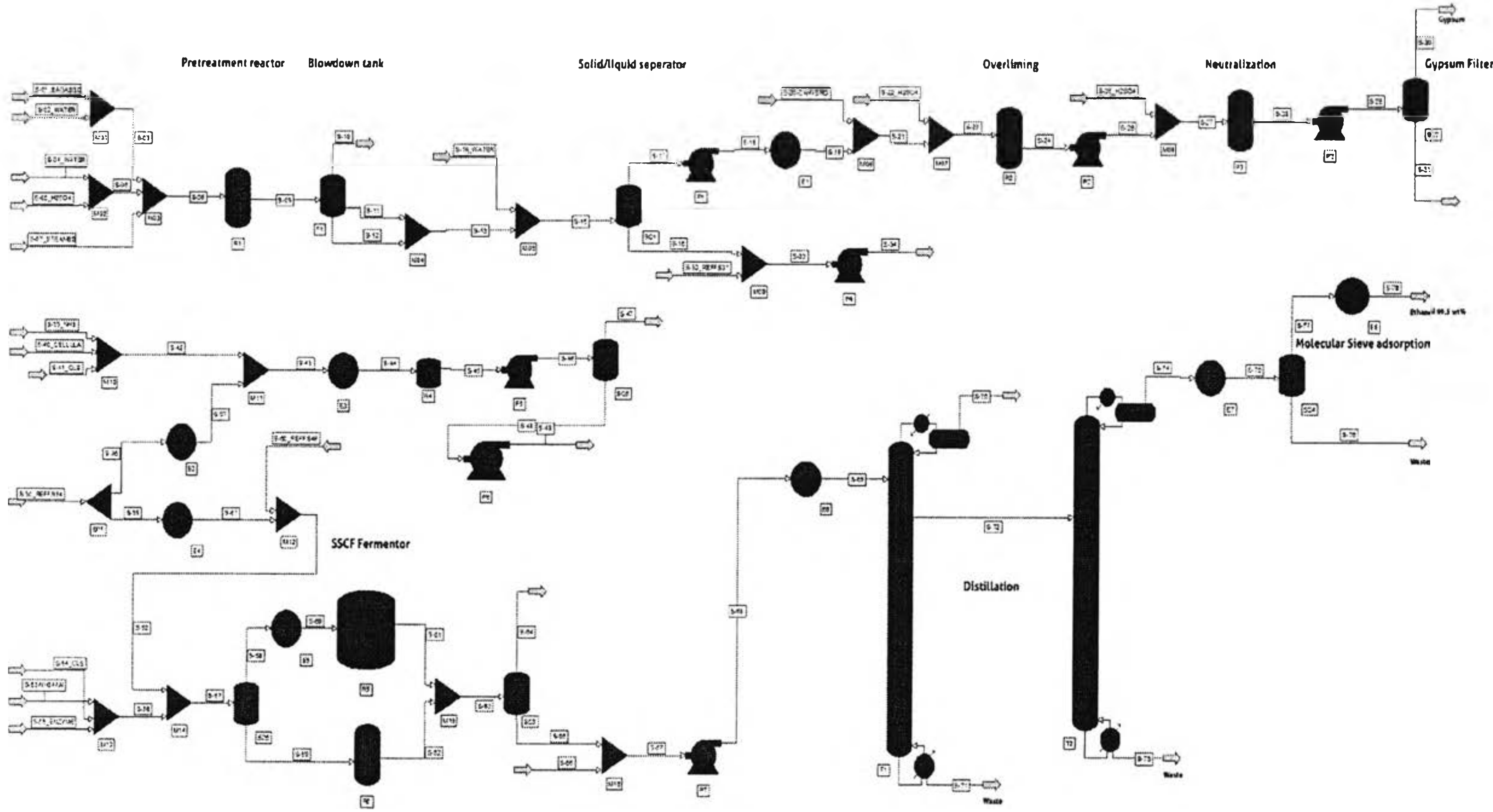

Figure C5 Flowsheet of the Alternative-4 implemented in PRO/II.

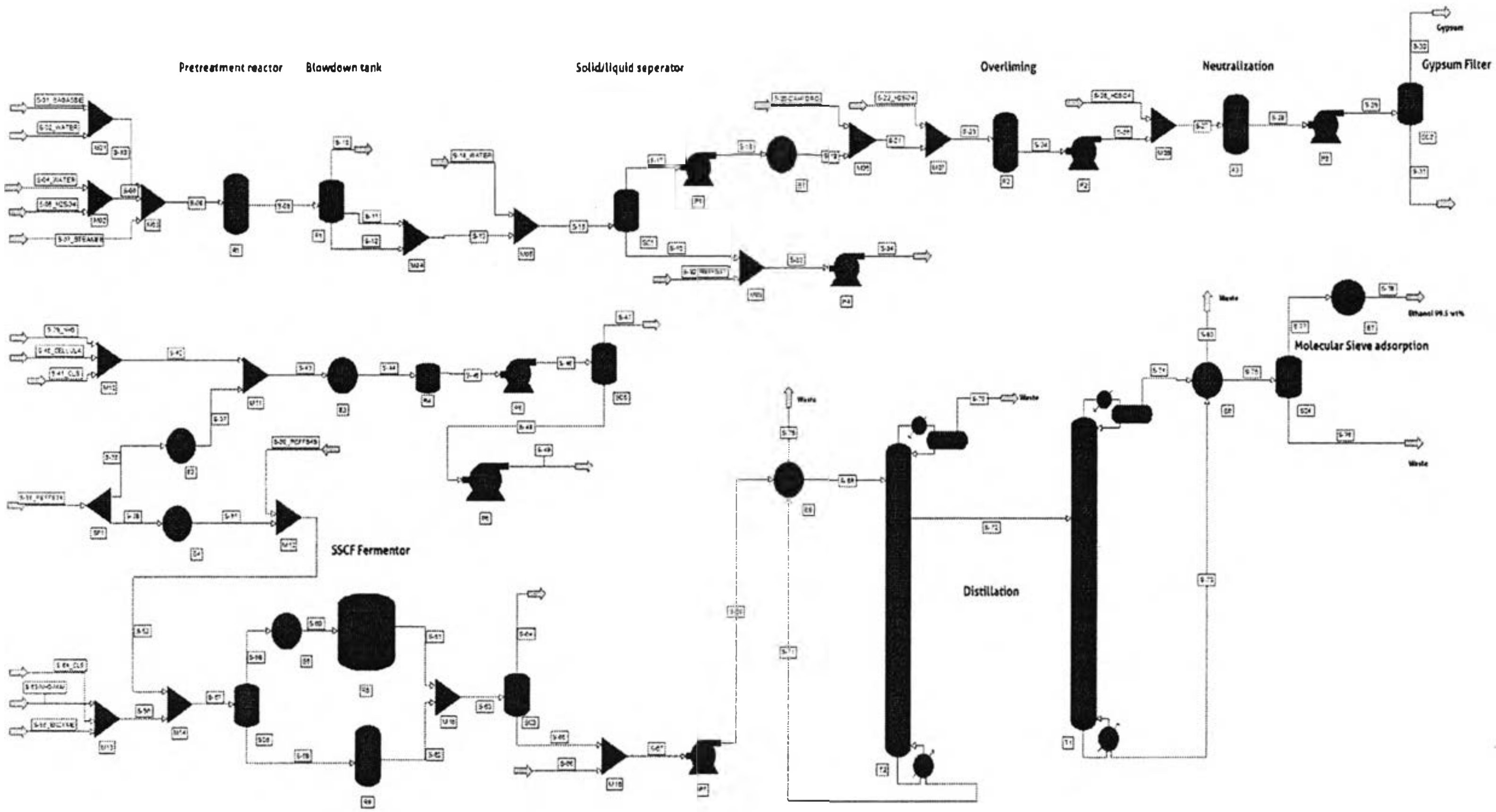

Figure C6 The process simulation of Alternatives-5.

Appendix D Stream Summary of The Base Case Design

Table D1 Stream summary of the base case design contemplating the streams S-01 until S-10

Stream Name		S-01	S-02	S-03	S-04	S-05	S-06	S-07	S-08	S-09	S-10
Phase		Mixed	Liquid	Mixed	Liquid	Liquid	Liquid	Vapor	Mixed	Mixed	Vapor
Temperature	°C	30	30	30	30	30	30	171	100	160	100
Pressure	atm	1	1	1	1	1	1	8	1	5	1
Total Enthalpy	GJ/h	-4	0	-4	0	0	0	9	5	19	4
Total Specific Enthalpy	kJ/kg	-797	126	-546	126	42	125	2773	473	1697	2680
Total Mass Rate	kg/h	5417	2020	7437	268	3	271	3333	11041	11041	1667
Total Molecular Weight	g/mol	31.2	18.0	26.0	18.0	98.1	18.2	18.0	22.7	23.0	18.0
Total Molar Rate	kg-mol/h	174	112	286	15	0	15	185	486	480	92
Component	M (g/mol)	Mass flow (kg/h)									
ETHANOL	46.1	0	0	0	0	0	0	0	0	0	0
WATER	18.0	2795	2020	4815	268	0	268	3333	8416	8317	1663
C6	180.2	0	0	0	0	0	0	0	0	84	0
C5	150.1	0	0	0	0	0	0	0	0	713	0
C5A	150.1	0	0	0	0	0	0	0	0	56	0
C6M	180.2	0	0	0	0	0	0	0	0	8	0
C12	342.3	0	0	0	0	0	0	0	0	8	0
CLS	18.0	0	0	0	0	0	0	0	0	0	0
ACETACID	60.1	0	0	0	0	0	0	0	0	0	0
SULFURIC	98.1	0	0	0	0	3	3	0	3	3	0
FURFURAL	96.1	0	0	0	0	0	0	0	0	5	3
HMF	126.1	0	0	0	0	0	0	0	0	0	0
CO2	44.0	0	0	0	0	0	0	0	0	0	0
O2	32.0	0	0	0	0	0	0	0	0	0	0
NH3	17.0	0	0	0	0	0	0	0	0	0	0
XYLITOL	152.2	0	0	0	0	0	0	0	0	0	0
LACACID	90.1	0	0	0	0	0	0	0	0	0	0
SUCCNAC	118.1	0	0	0	0	0	0	0	0	0	0
GLYCEROL	92.1	0	0	0	0	0	0	0	0	0	0
CELLULOS	162.1	1159	0	1159	0	0	0	0	1159	1076	0
HCELLULO	132.1	697	0	697	0	0	0	0	697	63	0
ARABINAN	132.1	55	0	55	0	0	0	0	55	5	0
MANNAN	162.1	8	0	8	0	0	0	0	8	1	0
CELLULAC	22.8	0	0	0	0	0	0	0	0	0	0
ZM	24.6	0	0	0	0	0	0	0	0	0	0
LIGNIN	122.5	703	0	703	0	0	0	0	703	703	0
CASO4	136.1	0	0	0	0	0	0	0	0	0	0
CAHYDROX	74.1	0	0	0	0	0	0	0	0	0	0

Table D2 Stream summary of the base case design contemplating the streams S-11 until S-20

Stream Name		S-11	S-12	S-13	S-14	S-15	S-16	S-17	S-18	S-19	S-20
Phase		Liquid	Solid	Mixed	Liquid	Mixed	Mixed	Mixed	Mixed	Mixed	Solid
Temperature	°C	100	100	100	30	72	72	72	72	50	30
Pressure	atm	1	1	1	1	1	1	1	1	1	1
Total Enthalpy	GJ/h	3	-3	0	1	1	-1	2	2	1	0
Total Specific Enthalpy	kJ/kg	422	-1665	11	126	51	-198	265	265	181	-2671
Total Mass Rate	kg/h	7527	1847	9374	5042	14416	6667	7750	7750	7750	20
Total Molecular Weight	g/mol	20.1	143.3	24.2	18.0	21.6	23.2	20.4	20.4	20.4	74.1
Total Molar Rate	kg-mol/h	375	13	388	280	668	288	380	380	380	0
Component	M (g/mol)	Mass flow (kg/h)									
ETHANOL	46.1	0	0	0	0	0	0	0	0	0	0
WATER	18.0	6653	0	6653	5042	11695	4974	6722	6722	6722	0
C6	180.2	84	0	84	0	84	1	83	83	83	0
C5	150.1	713	0	713	0	713	7	706	706	706	0
C5A	150.1	56	0	56	0	56	17	40	40	40	0
C6M	180.2	8	0	8	0	8	2	6	6	6	0
C12	342.3	8	0	8	0	8	2	6	6	6	0
CLS	18.0	0	0	0	0	0	0	0	0	0	0
ACETACID	60.1	0	0	0	0	0	0	0	0	0	0
SULFURIC	98.1	3	0	3	0	3	1	2	2	2	0
FURFURAL	96.1	2	0	2	0	2	1	1	1	1	0
HMF	126.1	0	0	0	0	0	0	0	0	0	0
CO2	44.0	0	0	0	0	0	0	0	0	0	0
O2	32.0	0	0	0	0	0	0	0	0	0	0
NH3	17.0	0	0	0	0	0	0	0	0	0	0
XYLITOL	152.2	0	0	0	0	0	0	0	0	0	0
LACACID	90.1	0	0	0	0	0	0	0	0	0	0
SUCCNAC	118.1	0	0	0	0	0	0	0	0	0	0
GLYCEROL	92.1	0	0	0	0	0	0	0	0	0	0
CELLULOS	162.1	0	1076	1076	0	1076	968	108	108	108	0
HCELLULO	132.1	0	63	63	0	63	56	6	6	6	0
ARABINAN	132.1	0	5	5	0	5	4	0	0	0	0
MANNAN	162.1	0	1	1	0	1	1	0	0	0	0
CELLULAC	22.8	0	0	0	0	0	0	0	0	0	0
ZM	24.6	0	0	0	0	0	0	0	0	0	0
LIGNIN	122.5	0	703	703	0	703	632	70	70	70	0
CASO4	136.1	0	0	0	0	0	0	0	0	0	0
CAHYDROX	74.1	0	0	0	0	0	0	0	0	0	20

Table D3 Stream summary of the base case design contemplating the streams S-21 until S-30

Stream Name		S-21	S-22	S-23	S-24	S-25	S-26	S-27	S-28	S-29	S-30
Phase		Mixed	Liquid	Mixed	Mixed	Mixed	Liquid	Mixed	Mixed	Mixed	Mixed
Temperature	°C	50	30	50	50	50	30	50	50	50	50
Pressure	atm	1	5	1	1	1	1	1	1	1	1
Total Enthalpy	GJ/h	1	0	1	1	1	0	1	1	1	0
Total Specific Enthalpy	kJ/kg	173	42	173	175	175	42	175	180	180	-1356
Total Mass Rate	kg/h	7770	5	7775	7775	7775	20	7794	7794	7794	153
Total Molecular Weight	g/mol	20.4	98.1	20.4	20.4	20.4	98.1	20.5	20.5	20.5	153.5
Total Molar Rate	kg-mol/h	380	0	380	380	380	0	381	381	381	1
Component	M (g/mol)	Mass flow (kg/h)									
ETHANOL	46.1	0	0	0	0	0	0	0	0	0	0
WATER	18.0	6722	0	6722	6724	6724	0	6724	6731	6731	0
C6	180.2	83	0	83	83	83	0	83	83	83	0
C5	150.1	706	0	706	706	706	0	706	706	706	1
C5A	150.1	40	0	40	40	40	0	40	40	40	0
C6M	180.2	6	0	6	6	6	0	6	6	6	0
C12	342.3	6	0	6	6	6	0	6	6	6	0
CLS	18.0	0	0	0	0	0	0	0	0	0	0
ACETACID	60.1	0	0	0	0	0	0	0	0	0	0
SULFURIC	98.1	2	5	7	0	0	20	20	0	0	0
FURFURAL	96.1	1	0	1	1	1	0	1	1	1	0
HMF	126.1	0	0	0	0	0	0	0	0	0	0
CO2	44.0	0	0	0	0	0	0	0	0	0	0
O2	32.0	0	0	0	0	0	0	0	0	0	0
NH3	17.0	0	0	0	0	0	0	0	0	0	0
XYLITOL	152.2	0	0	0	0	0	0	0	0	0	0
LACACID	90.1	0	0	0	0	0	0	0	0	0	0
SUCCNAC	118.1	0	0	0	0	0	0	0	0	0	0
GLYCEROL	92.1	0	0	0	0	0	0	0	0	0	0
CELLULOS	162.1	108	0	108	108	108	0	108	108	108	108
HCELLULO	132.1	6	0	6	6	6	0	6	6	6	6
ARABINAN	132.1	0	0	0	0	0	0	0	0	0	0
MANNAN	162.1	0	0	0	0	0	0	0	0	0	0
CELLULAC	22.8	0	0	0	0	0	0	0	0	0	0
ZM	24.6	0	0	0	0	0	0	0	0	0	0
LIGNIN	122.5	70	0	70	70	70	0	70	70	70	0
CASO4	136.1	0	0	0	10	10	0	10	37	37	37
CAHYDROX	74.1	20	0	20	15	15	0	15	0	0	0

Table D4 Stream summary of the base case design contemplating the streams S-31 until S-40

Stream Name		S-31	S-32	S-33	S-34	S-35	S-36	S-37	S-38	S-39	S-40
Phase		Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Vapor	Mixed
Temperature	°C	50	50	60	60	60	60	30	60	30	30
Pressure	atm	1	1	1	1	1	1	1	1	1	1
Total Enthalpy	GJ/h	2	2	0	0	0	0	0	0	0	0
Total Specific Enthalpy	kJ/kg	210	210	20	20	20	20	-88	20	1283	107
Total Mass Rate	kg/h	7641	7641	14308	14308	14308	1431	1431	12877	0	117
Total Molecular Weight	g/mol	20.1	20.1	21.4	21.4	21.4	21.4	21.4	21.4	17.0	18.1
Total Molar Rate	kg-mol/h	380	380	668	668	668	67	67	601	0	6
Component	M (g/mol)	Mass flow (kg/h)									
ETHANOL	46.1	0	0	0	0	0	0	0	0	0	0
WATER	18.0	6731	6731	11705	11705	11705	1171	1171	10535	0	116
C6	180.2	83	83	84	84	84	8	8	75	0	0
C5	150.1	705	705	712	712	712	71	71	641	0	0
C5A	150.1	40	40	56	56	56	6	6	51	0	0
C6M	180.2	6	6	8	8	8	1	1	7	0	0
C12	342.3	6	6	8	8	8	1	1	7	0	0
CLS	18.0	0	0	0	0	0	0	0	0	0	0
ACETACID	60.1	0	0	0	0	0	0	0	0	0	0
SULFURIC	98.1	0	0	1	1	1	0	0	1	0	0
FURFURAL	96.1	1	1	2	2	2	0	0	2	0	0
HMF	126.1	0	0	0	0	0	0	0	0	0	0
CO2	44.0	0	0	0	0	0	0	0	0	0	0
O2	32.0	0	0	0	0	0	0	0	0	0	0
NH3	17.0	0	0	0	0	0	0	0	0	0	0
XYLITOL	152.2	0	0	0	0	0	0	0	0	0	0
LACACID	90.1	0	0	0	0	0	0	0	0	0	0
SUCCNAC	118.1	0	0	0	0	0	0	0	0	0	0
GLYCEROL	92.1	0	0	0	0	0	0	0	0	0	0
CELLULOS	162.1	0	0	968	968	968	97	97	871	0	0
HCELLULO	132.1	0	0	56	56	56	6	6	51	0	0
ARABINAN	132.1	0	0	4	4	4	0	0	4	0	0
MANNAN	162.1	0	0	1	1	1	0	0	1	0	0
CELLULAC	22.8	0	0	0	0	0	0	0	0	0	2
ZM	24.6	0	0	0	0	0	0	0	0	0	0
LIGNIN	122.5	70	70	703	703	703	70	70	632	0	0
CASO4	136.1	0	0	0	0	0	0	0	0	0	0
CAHYDROX	74.1	0	0	0	0	0	0	0	0	0	0

Table D5 Stream summary of the base case design contemplating the streams S-41 until S-50

Stream Name		S-41	S-42	S-43	S-44	S-45	S-46	S-47	S-48	S-49	S-50
Phase		Liquid	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed	Mixed
Temperature	°C	30	30	30	30	30	30	29	29	29	29
Pressure	atm	1	1	1	1	1	1	1	1	1	1
Total Enthalpy	GJ/h	0	0	0	0	0	0	0	0	0	0
Total Specific Enthalpy	kJ/kg	126	110	-71	-71	-58	-58	215	-65	-65	-65
Total Mass Rate	kg/h	19	136	1567	1567	1567	1567	39	1528	1528	1528
Total Molecular Weight	g/mol	18.0	18.1	21.1	21.1	20.8	20.8	43.0	20.5	20.5	20.5
Total Molar Rate	kg-mol/h	1	8	74	74	76	76	1	75	75	75
Component	M (g/mol)	Mass flow (kg/h)									
ETHANOL	46.1	0	0	0	0	42	42	0	42	42	42
WATER	18.0	0	116	1286	1286	1284	1284	1	1283	1283	1283
C6	180.2	0	0	8	8	4	4	0	4	4	4
C5	150.1	0	0	71	71	13	13	0	13	13	13
C5A	150.1	0	0	6	6	6	6	0	6	6	6
C6M	180.2	0	0	1	1	1	1	0	1	1	1
C12	342.3	0	0	1	1	1	1	0	1	1	1
CLS	18.0	19	19	19	19	19	19	0	19	19	19
ACETACID	60.1	0	0	0	0	0	0	0	0	0	0
SULFURIC	98.1	0	0	0	0	0	0	0	0	0	0
FURFURAL	96.1	0	0	0	0	0	0	0	0	0	0
HMF	126.1	0	0	0	0	0	0	0	0	0	0
CO2	44.0	0	0	0	0	40	40	38	2	2	2
O2	32.0	0	0	0	0	0	0	0	0	0	0
NH3	17.0	0	0	0	0	0	0	0	0	0	0
XYLITOL	152.2	0	0	0	0	0	0	0	0	0	0
LACACID	90.1	0	0	0	0	0	0	0	0	0	0
SUCCNAC	118.1	0	0	0	0	0	0	0	0	0	0
GLYCEROL	92.1	0	0	0	0	0	0	0	0	0	0
CELLULOS	162.1	0	0	97	97	77	77	0	77	77	77
HCELLULO	132.1	0	0	6	6	6	6	0	6	6	6
ARABINAN	132.1	0	0	0	0	0	0	0	0	0	0
MANNAN	162.1	0	0	0	0	0	0	0	0	0	0
CELLULAC	22.8	0	2	2	2	2	2	0	2	2	2
ZM	24.6	0	0	0	0	0	0	0	0	0	0
LIGNIN	122.5	0	0	70	70	70	70	0	70	70	70
CASO4	136.1	0	0	0	0	0	0	0	0	0	0
CAHYDROX	74.1	0	0	0	0	0	0	0	0	0	0

Table D6 Stream summary of the base case design contemplating the streams S-51 until S-60

Stream Name		S-51	S-52	S-53	S-54	S-55	S-56	S-57	S-58	S-59	S-60
Phase		Mixed	Mixed	Vapor	Liquid	Mixed	Mixed	Mixed	Mixed	Liquid	Mixed
Temperature	°C	30	30	30	30	30	30	30	30	30	30
Pressure	atm	1	1	1	1	1	1	1	1	1	1
Total Enthalpy	GJ/h	-1	-1	0	0	0	0	-1	-1	0	-1
Total Specific Enthalpy	kJ/kg	-88	-86	1283	126	102	103	-74	-75	349	-75
Total Mass Rate	kg/h	12877	14405	0	30	975	1005	15410	15354	56	15354
Total Molecular Weight	g/mol	21.4	21.3	17.0	18.0	18.1	18.1	21.1	21.0	152.9	21.0
Total Molar Rate	kg-mol/h	601	675	0	2	54	56	731	731	0	731
Component	M (g/mol)	Mass flow (kg/h)									
ETHANOL	46.1	0	42	0	0	0	0	42	42	0	42
WATER	18.0	10535	11818	0	0	955	955	12773	12773	0	12773
C6	180.2	75	79	0	0	0	0	79	74	6	74
C5	150.1	641	654	0	0	0	0	654	608	46	608
C5A	150.1	51	56	0	0	0	0	56	52	4	52
C6M	180.2	7	8	0	0	0	0	8	7	1	7
C12	342.3	7	8	0	0	0	0	8	8	0	8
CLS	18.0	0	19	0	30	0	30	49	49	0	49
ACETACID	60.1	0	0	0	0	0	0	0	0	0	0
SULFURIC	98.1	1	1	0	0	0	0	1	1	0	1
FURFURAL	96.1	2	2	0	0	0	0	2	2	0	2
HMF	126.1	0	0	0	0	0	0	0	0	0	0
CO2	44.0	0	2	0	0	0	0	2	2	0	2
O2	32.0	0	0	0	0	0	0	0	0	0	0
NH3	17.0	0	0	0	0	0	0	0	0	0	0
XYLITOL	152.2	0	0	0	0	0	0	0	0	0	0
LACACID	90.1	0	0	0	0	0	0	0	0	0	0
SUCCNAC	118.1	0	0	0	0	0	0	0	0	0	0
GLYCEROL	92.1	0	0	0	0	0	0	0	0	0	0
CELLULOS	162.1	871	949	0	0	0	0	949	949	0	949
HCELLULO	132.1	51	56	0	0	0	0	56	56	0	56
ARABINAN	132.1	4	4	0	0	0	0	4	4	0	4
MANNAN	162.1	1	1	0	0	0	0	1	1	0	1
CELLULAC	22.8	0	2	0	0	19	19	21	21	0	21
ZM	24.6	0	0	0	0	0	0	0	0	0	0
LIGNIN	122.5	632	703	0	0	0	0	703	703	0	703
CASO4	136.1	0	0	0	0	0	0	0	0	0	0
CAHYDROX	74.1	0	0	0	0	0	0	0	0	0	0

Table D7 Stream summary of the base case design contemplating the streams S-61 until S-70

Stream Name		S-61	S-62	S-63	S-64	S-65	S-66	S-67	S-68	S-69	S-70
Phase		Mixed	Liquid	Mixed	Mixed	Mixed	Liquid	Mixed	Mixed	Mixed	Mixed
Temperature	°C	30	30	30	29	29	30	30	90	95	82
Pressure	atm	1	1	1	1	1	1	1	1	1	1
Total Enthalpy	GJ/h	0	0	0	0	0	5	5	20	21	18
Total Specific Enthalpy	kJ/kg	12	69	12	226	3	121	92	334	360	308
Total Mass Rate	kg/h	15354	56	15410	675	14735	44850	59585	59585	57367	56934
Total Molecular Weight	g/mol	20.5	90.1	20.6	43.0	20.1	19.0	19.2	19.2	18.5	18.4
Total Molar Rate	kg-mol/h	748	1	749	16	733	2366	3100	3100	3099	3097
Component	M (g/mol)	Mass flow (kg/h)									
ETHANOL	46.1	743	0	743	10	732	3640	4373	4373	762	124
WATER	18.0	12689	0	12689	11	12678	41209	53887	53887	55298	55500
C6	180.2	69	0	69	0	69	0	69	69	69	69
C5	150.1	84	0	84	0	84	0	84	84	84	84
C5A	150.1	52	0	52	0	52	0	52	52	52	52
C6M	180.2	7	0	7	0	7	0	7	7	7	7
C12	342.3	0	0	0	0	0	0	0	0	0	0
CLS	18.0	49	0	49	0	49	0	49	49	51	54
ACETACID	60.1	4	0	4	0	4	0	4	4	4	4
SULFURIC	98.1	1	0	1	0	1	0	1	1	1	1
FURFURAL	96.1	2	0	2	0	2	0	2	2	1	0
HMF	126.1	0	0	0	0	0	0	0	0	0	0
CO2	44.0	671	0	671	652	19	0	19	19	0	0
O2	32.0	1	0	1	1	0	0	0	0	0	0
NH3	17.0	0	0	0	0	0	0	0	0	0	0
XYLITOL	152.2	1	0	1	0	1	0	1	1	1	1
LACACID	90.1	2	56	58	0	58	0	58	58	58	58
SUCCNAC	118.1	2	0	2	0	2	0	2	2	2	2
GLYCEROL	92.1	1	0	1	0	1	0	1	1	1	1
CELLULOS	162.1	188	0	188	0	188	0	188	188	188	188
HCELLULO	132.1	56	0	56	0	56	0	56	56	56	56
ARABINAN	132.1	4	0	4	0	4	0	4	4	4	4
MANNAN	162.1	1	0	1	0	1	0	1	1	1	1
CELLULAC	22.8	21	0	21	0	21	0	21	21	21	21
ZM	24.6	4	0	4	0	4	0	4	4	4	4
LIGNIN	122.5	703	0	703	0	703	0	703	703	703	703
CASO4	136.1	0	0	0	0	0	0	0	0	0	0
CAHYDROX	74.1	0	0	0	0	0	0	0	0	0	0

Table D8 Stream summary of the base case design contemplating the streams S-71 until S-80

Stream Name		S-71	S-72	S-73	S-74	S-75	S-76	S-77	S-78	S-79	S-80
Phase		Mixed	Mixed	Vapor	Vapor	Vapor	Vapor	Mixed	Liquid	Vapor	Vapor
Temperature	°C	52	49	49	52	82	95	98	100	79	95
Pressure	atm	0	0	0	0	1	1	1	1	1	1
Total Enthalpy	GJ/h	10	4	71	72	74	75	75	11	6	6
Total Specific Enthalpy	kJ/kg	185	144	2590	2589	2609	2443	2440	419	1224	1247
Total Mass Rate	kg/h	56407	28806	27602	27950	28384	30598	30598	25638	4960	4960
Total Molecular Weight	g/mol	18.4	18.7	18.0	18.1	18.3	19.7	19.7	18.0	39.0	39.0
Total Molar Rate	kg-mol/h	3071	1540	1531	1547	1550	1550	1550	1423	127	127
Component	M (g/mol)	Mass flow (kg/h)									
ETHANOL	46.1	20	2	19	123	760	4370	4370	4	4366	4366
WATER	18.0	55075	27517	27558	27806	27604	26190	26190	25616	574	574
C6	180.2	69	69	0	0	0	0	0	0	0	0
C5	150.1	84	84	0	0	0	0	0	0	0	0
C5A	150.1	52	52	0	0	0	0	0	0	0	0
C6M	180.2	7	7	0	0	0	0	0	0	0	0
C12	342.3	0	0	0	0	0	0	0	0	0	0
CLS	18.0	58	35	23	19	16	14	14	14	0	0
ACETACID	60.1	3	1	2	3	3	3	3	3	0	0
SULFURIC	98.1	1	1	0	0	0	0	0	0	0	0
FURFURAL	96.1	0	0	0	0	1	2	2	1	1	1
HMF	126.1	0	0	0	0	0	0	0	0	0	0
CO2	44.0	0	0	0	0	0	19	19	0	19	19
O2	32.0	0	0	0	0	0	0	0	0	0	0
NH3	17.0	0	0	0	0	0	0	0	0	0	0
XYLITOL	152.2	1	1	0	0	0	0	0	0	0	0
LACACID	90.1	58	58	0	0	0	0	0	0	0	0
SUCCNAC	118.1	2	2	0	0	0	0	0	0	0	0
GLYCEROL	92.1	1	1	0	0	0	0	0	0	0	0
CELLULOS	162.1	188	188	0	0	0	0	0	0	0	0
HCELLULO	132.1	56	56	0	0	0	0	0	0	0	0
ARABINAN	132.1	4	4	0	0	0	0	0	0	0	0
MANNAN	162.1	1	1	0	0	0	0	0	0	0	0
CELLULAC	22.8	21	21	0	0	0	0	0	0	0	0
ZM	24.6	4	4	0	0	0	0	0	0	0	0
LIGNIN	122.5	703	703	0	0	0	0	0	0	0	0
CASO4	136.1	0	0	0	0	0	0	0	0	0	0
CAHYDROX	74.1	0	0	0	0	0	0	0	0	0	0

Table D9 Stream summary of the base case design contemplating the streams S-81 until S-82

Stream Name		S-81	S-82	S-83
Phase		Mixed	Vapor	Liquid
Temperature	°C	100	100	32
Pressure	atm	1	1	1
Total Enthalpy	GJ/h	2	5	0
Total Specific Enthalpy	kJ/kg	2547	1071	76
Total Mass Rate	kg/h	591	4369	4369
Total Molecular Weight	g/mol	18.4	46.0	46.0
Total Molar Rate	kg-mol/h	32	95	95
Component	M (g/mol)	Mass flow (kg/h)		
ETHANOL	46.1	0	4366	4366
WATER	18.0	571	3	3
C6	180.2	0	0	0
C5	150.1	0	0	0
C5A	150.1	0	0	0
C6M	180.2	0	0	0
C12	342.3	0	0	0
CLS	18.0	0	0	0
ACETACID	60.1	0	0	0
SULFURIC	98.1	0	0	0
FURFURAL	96.1	1	0	0
HMF	126.1	0	0	0
CO2	44.0	19	0	0
O2	32.0	0	0	0
NH3	17.0	0	0	0
XYLITOL	152.2	0	0	0
LACACID	90.1	0	0	0
SUCCNAC	118.1	0	0	0
GLYCEROL	92.1	0	0	0
CELLULOS	162.1	0	0	0
HCELLULO	132.1	0	0	0
ARABINAN	132.1	0	0	0
MANNAN	162.1	0	0	0
CELLULAC	22.8	0	0	0
ZM	24.6	0	0	0
LIGNIN	122.5	0	0	0
CASO4	136.1	0	0	0
CAHYDROX	74.1	0	0	0

Appendix E Stage Model and Result from GAMS of Alternative-4

```
SETS
    I  hot streams /I1,I2,I3,I4,I5,I6/
    J  cold streams /J1,J2/
    K  Stage no. /K1,K2,K3/;

PARAMETER TINI(I) /I1=72.25, I2=59.83, I3=59.83, I4=99.99, I5=120.73, I6=100.02/

        TINJ(J) /J1=29.94, J2=78.71/

        TOUTI(I)/I1=50, I2=30, I3=30, I4=32, I5=40.57, I6=40.57/

        TOUTJ(J)/J1=100, J2=95/

        FI(I)  /I1=8.1461, I2=1.4471, I3=13.0201, I4=17.6599, I5=58.3039, I6=4.7679/

        FJ(J)  /J1=66.715, J2=1.874/

        OMEGA  /1000000/
        TAL    /1000000/
        EMAT   /1.8/;


VARIABLES
    dt(I,J,K)  Approach temperature
    dtcu(I)   Approach temperature between cold utility and hot stream
    dthu(J)   Approach temperature between hot utility and cold stream
    q(I,J,K)  heat exchanged between hot I and cold J
    qcu(I)    heat exchanged between cold utility and hot I
    qhu(J)    heat exchanged between hot utility and cold J
    ti(I,K)   temp of hot stream i at hot end of stage k
    tj(J,K)   temp of cold stream j at hot end of stage k
    z(I,J,K)  exchanger matching between hot I and cold J at stage k
    zcu(I)    cold utility matching with hot I
    zhu(J)    hot utility matching with cold J
    ZZ        total energy
    dtt(I,J,K) actual temperature;

POSITIVE VARIABLE dt(I,J,K),dtcu(I),dthu(J),q(I,J,K),qcu(I),qhu(J),tj(J,K),ti(I,K);
BINARY VARIABLES  zcu(I),zhu(J),z(I,J,K);


EQUATIONS


    MINU          objective function minimize utilities

    HOTI(I)       heat balance in hot streams I
    COLDJ(J)        heat balance in cold stream J

    HOTK1(I)        heat balance of hot  at stage K1
    HOTK2(I)        heat balance of hot  at stage K2


    COLDK1(J)        heat balance of cold  at stage K1
    COLDK2(J)        heat balance of cold  at stage K2


    TINHOT(I)       hot temp in
    TINCOLD(J)        cold temp in

    FEHOTK1(I)        feasibility of  hot temp   at stage K1
    FEHOTK2(I)        feasibility of  hot temp   at stage K2

    FECOLDK1(J)        feasibility of  cold temp  at stage K1
```

Figure E1 Stage model of Alternative-4 added to GAMS (1)

```
    FECOLDK2(J)        feasibility of  cold temp  at stage K2


    FEHOTOUT(I)        feasibility of  hot temp out
    FECOLDOUT(J)        feasibility of  cold temp out

    HOTU(I)          hot utility load
    COLDU(J)          cold utility load

    LogicK1(I,J)      Logical constraint at stage k1
    LogicK2(I,J)      Logical constraint at stage k2


    LogicHOT(J)       Logical constraint hot  utility
    LogicCOLD(I)       Logical constraint cold utility

    ApproK1(I,J)      approach temp at stage k1
    AApproK1(I,J)      the other approach temp at stage k1
    ApproK2(I,J)      approach temp at stage k2
    AApproK2(I,J)      the other approach temp at stage k2

    EMATdt1(I,J,K)     EMAT constraint

    CONSTRAINT1        constraint  no.1
    CONSTRAINT2        constraint  no.2
    CONSTRAINT3        constraint  no.3
    CONSTRAINT4        constraint  no.4
    CONSTRAINT5        constraint  no.5
    CONSTRAINT6        constraint  no.6
    CONSTRAINT7        constraint  no.7;


MINU      .. ZZ  =E= 8*SUM(I,qcu(I)) + 341*SUM(J,qhu(J))
              +10*SUM((I,J,K),z(I,J,K))
              +10*SUM(I,zcu(I))+ 10*SUM(J,zhu(J));

HOTI(I)   .. (TINI(I)-TOUTI(I))*FI(I)=E= SUM((J,K),q(I,J,K))+qcu(I);
COLDJ(J)  .. (TOUTJ(J)-TINJ(J))*FJ(J)=E= SUM((I,K),q(I,J,K))+qhu(J);

HOTK1(I)  .. (ti(I,'K1')-ti(I,'K2'))*FI(I)=E= SUM(J,q(I,J,'K1'));
HOTK2(I)  .. (ti(I,'K2')-ti(I,'K3'))*FI(I)=E= SUM(J,q(I,J,'K2'));

COLDK1(J) .. (tj(J,'K1')-tj(J,'K2'))*FJ(J)=E= SUM(I,q(I,J,'K1'));
COLDK2(J) .. (tj(J,'K2')-tj(J,'K3'))*FJ(J)=E= SUM(I,q(I,J,'K2'));

TINHOT(I) .. TINI(I) =E= ti(I,'K1');
TINCOLD(J) .. TINJ(J) =E= tj(J,'K3');

FEHOTK1(I) .. ti(I,'K1') =G= ti(I,'K2');
FEHOTK2(I) .. ti(I,'K2') =G= ti(I,'K3');

FECOLDK1(J) .. tj(J,'K1') =G= tj(J,'K2');
FECOLDK2(J) .. tj(J,'K2') =G= tj(J,'K3');

FEHOTOUT(I) .. TOUTI(I) =L= ti(I,'K3');
FECOLDOUT(J).. TOUTJ(J) =G= tj(J,'K1');

HOTU(I)  .. (ti(I,'K3')-TOUTI(I))*FI(I) =E= qcu(I);
COLDU(J) .. (TOUTJ(J)-tj(j,'K1'))*FJ(J) =E= qhu(J);

LogicK1(I,J)  .. q(I,J,'K1')-OMEGA*z(I,J,'K1') =L= 0;
LogicK2(I,J)  .. q(I,J,'K2')-OMEGA*z(I,J,'K2') =L= 0;

LogicHOT(J) .. qhu(J)-OMEGA*zhu(J) =L= 0;
LogicCOLD(I).. qcu(I)-OMEGA*zcu(I) =L= 0;
```

Figure E2 Stage model of Alternative-4 added to GAMS (2, cont.)

```
ApproK1(I,J) .. dt(I,J,'K1') =L= (ti(I,'K1')-tj(J,'K1'))+TAL*(1-z(I,J,'K1'));
AApproK1(I,J) .. dt(I,J,'K2') =L= (ti(I,'K2')-tj(J,'K2'))+TAL*(1-z(I,J,'K1'));
ApproK2(I,J) .. dt(I,J,'K2') =L= (ti(I,'K2')-tj(J,'K2'))+TAL*(1-z(I,J,'K2'));
AApproK2(I,J) .. dt(I,J,'K3') =L= (ti(I,'K3')-tj(J,'K3'))+TAL*(1-z(I,J,'K2'));

EMATdt1(I,J,K) .. dt(I,J,K) =G= EMAT;

CONSTRAINT1 .. sum(J,qhu(J)) =L= 4704.5837;
CONSTRAINT2 .. qcu('I1') =E= 181.25;
CONSTRAINT3 .. qcu('I2') =E= 43.1667;
CONSTRAINT4 .. qcu('I3') =E= 388.3889;
CONSTRAINT5 .. qcu('I4') =E= 1200.6945;
CONSTRAINT6 .. qcu('I5') =E= 0;
CONSTRAINT7 .. qhu('J1') =E= 0;

MODEL TSHIP /ALL/ ;
SOLVE TSHIP USING MIP MINIMIZING ZZ;
DISPLAY ZZ.L,dt.L,ti.L,tj.L,z.L,zcu.L,zhu.L,q.L,qcu.L,qhu.L;
```

Figure E3 Stage model of Alternative-4 added to GAMS (3, cont.)

```
----   149 VARIABLE z.L  exchanger matching between hot I and cold J at stage k

          K1        K2

I1.J1               1.000
I2.J1               1.000
I3.J1               1.000
I4.J2     1.000
I5.J1     1.000
I6.J1               1.000
I6.J2     1.000


----   149 VARIABLE zcu.L  cold utility matching with hot I

I1 1.000,   I2 1.000,   I3 1.000,   I4 1.000,   I6 1.000


----   149 VARIABLE zhu.L  hot utility matching with cold J

              ( ALL      0.000 )


----   149 VARIABLE q.L  heat exchanged between hot I and cold J

          K1        K2

I1.J1          7.250000E-4
I2.J1          2.930000E-4
I3.J1          6.830000E-4
I4.J2     0.002
I5.J1  4673.641
I6.J1               0.411
I6.J2    30.525

----   149 VARIABLE qcu.L  heat exchanged between cold utility and hot I

I1  181.250,   I2  43.167,   I3  388.389,   I4 1200.694,   I6  252.516

----   149 VARIABLE qhu.L  heat exchanged between hot utility and cold J

              ( ALL      0.000 )
```

Figure E4 Result of stage model of Alternative-4 from GAMS

Appendix F Life Cycle Inventory Analysis of New Design Alternatives

F.1 Alternative-1

Table F1.1 List of inventory of Alternative-1 in Pretreatment stage

Input Inventory			Output Inventory		
Type	**Amount**	**Unit**	**Type**	**Amount**	**Unit**
Material			***Product***		
Sulphuric acid	0.0037	Kg	Output-1 from Pretreatment Stage	12.8198	Kg
Utilities			***Emission to Air***		
Water	3.1292	Kg	Water	2.2747	Kg
			Furfural	0.0046	Kg
Energy					
Steam	12.6961	Kg			

Table F1.2 List of inventory of Alternative-1 in Neutralization stage

Input Inventory			Output Inventory		
Type	**Amount**	**Unit**	**Type**	**Amount**	**Unit**
Material			***Product***		
Output-1 from Pretreatment Stage	12.8198	Kg	Output-2 from Neutralization Stage	19.5670	Kg
Sulphuric acid	0.0336	Kg			
Calcium hydroxide	0.0274	Kg	***Solid Waste***		
			Gypsum	0.0502	Kg
Utilities			Glucose	0.0002	Kg
Water	6.8953	Kg	Xylose	0.0019	Kg
			Arabinose	0.0001	Kg
Energy			Cellulose	0.1471	Kg
Electricity	0.0002	KWh	Hemicellulose	0.0086	Kg
			Arabinan	0.0007	Kg
			Mannan	0.0001	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***		
Output-2 from neutralization stage	19.5670	Kg	Output-3 from fermentation stage	20.1513	Kg
Ammonia	0.0006	Kg			
Cellulase	0.0025	Kg	***Emission to Air***		
Corn steep liquor	0.0665	Kg	Water	0.0165	Kg
Zymomonas Mobilis	0.0262	Kg	Ethanol	0.0148	Kg
			Carbondioxide	0.9440	Kg
Utilities			Oxygen	0.0010	Kg
Water	1.4647	Kg			
Energy					
Electricity	0.00002	KWh			

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-3 from Fermentation Stage	20.1513	Kg		Ethanol 99.5 wt%	1.0000	Kg
Energy						
Electricity	0.0091	KWh		***Liquid waste***		
Steam	13.1788	Kg		Waste water	19.0417	Kg

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

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Waste water	19.0417	Kg		Steam	3.7035	Kg
				Electricity	0.9811	KWh
				Emission to air		
				Nitrogen oxides	1.77E-04	Kg
				Carbon monoxide	5.66E-04	Kg
				Methane, biogenic	2.71E-04	Kg
				NMVOC	2.36E-05	Kg
				Dinitrogen monoxide	2.95E-05	Kg
				Sulfur dioxide	2.48E-04	Kg
				Platinum	8.25E-11	Kg
				Heat, waste	1.04E+01	MJ
				Used mineral oil, to waste inceneration	3.54E-04	Kg

F.2 Alternative-2

Table F2.1 List of inventory of Alternative-2 in Pretreatment stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Sulphuric acid	0.0037	Kg		Output-1 from Pretreatment Stage	12.8413	Kg
Utilities				***Emission to Air***		
Water	3.1344	Kg		Water	2.2785	Kg
				Furfural	0.0046	Kg
Energy						
Steam	12.7175	Kg				

Table F2.2 List of inventory of Alternative-2 in Neutralization stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Output-1 from Pretreatment Stage	12.8413	Kg		Output-2 from Neutralization Stage	19.5999	Kg
Sulphuric acid	0.0337	Kg				
Calcium hydroxide	0.0274	Kg		***Solid Waste***		
				Gypsum	0.0503	Kg
Utilities				Glucose	0.0002	Kg
Water	6.9069	Kg		Xylose	0.0019	Kg
				Arabinose	0.0001	Kg
Energy				Cellulose	0.1474	Kg
Electricity	0.0002	KWh		Hemicellulose	0.0086	Kg
				Arabinan	0.0007	Kg
				Mannan	0.0001	Kg

Table F2.3 List of inventory of Alternative-2 in Fermentation stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Output-2 from neutralization stage	19.5999	Kg		Output-3 from fermentation stage	20.1852	Kg
Ammonia	0.0006	Kg				
Cellulase	0.0025	Kg		***Emission to Air***		
Corn steep liquor	0.07	Kg		Water	0.0165	Kg
Zymomonas Mobilis	0.0262	Kg		Ethanol	0.0148	Kg
				Carbondioxide	0.9456	Kg
Utilities				Oxygen	0.0010	Kg
Water	1.4672	Kg				
Energy						
Electricity	0.00002	KWh				

Table F2.4 List of inventory of Alternative-2 in recovery stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Output-3 from Fermentation Stage	20.1852	Kg		Ethanol 99.5 wt%	1.0000	Kg
Energy						
Electricity	0.0186	KWh		***Liquid waste***		
Steam	12.6095	Kg		Waste water	19.0655	Kg

Table F2.5 List of inventory of Alternative-2 in biogas and cogeneration stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				*Product*		
Waste water	19.0655	Kg		Steam	3.6624	Kg
				Electricity	0.9702	KWh
				Emission to air		
				Nitrogen oxides	1.75E-04	Kg
				Carbon monoxide	5.60E-04	Kg
				Methane, biogenic	2.68E-04	Kg
				NMVOC	2.33E-05	Kg
				Dinitrogen monoxide	2.91E-05	Kg
				Sulfur dioxide	2.45E-04	Kg
				Platinum	8.16E-11	Kg
				Heat, waste	1.03E+01	MJ
				Used mineral oil, to waste inceneration	3.50E-04	Kg

F.3 Alternative-3

Table F3.1 List of inventory of Alternative-3 in Pretreatment stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				*Product*		
Sulphuric acid	0.0037	Kg		Output-1 from Pretreatment Stage	12.8110	Kg
Utilities				*Emission to Air*		
Water	3.1270	Kg		Water	2.2731	Kg
				Furfural	0.0046	Kg
Energy						
Steam	12.6874	Kg				

Table F3.2 List of inventory of Alternative-3 in Neutralization stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				*Product*		
Output-1 from Pretreatment Stage	12.8110	Kg		Output-2 from Neutralization Stage	19.5535	Kg
Sulphuric acid	0.0336	Kg				
Calcium hydroxide	0.0273	Kg		*Solid Waste*		
				Gypsum	0.0502	Kg
Utilities				Glucose	0.0002	Kg
Water	6.8906	Kg		Xylose	0.0019	Kg
				Arabinose	0.0001	Kg
Energy				Cellulose	0.1470	Kg
Electricity	0.0002	KWh		Hemicellulose	0.0086	Kg
				Arabinan	0.0007	Kg
				Mannan	0.0001	Kg

Table F3.3 List of inventory of Alternative-3 in Fermentation stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Output-2 from neutralization stage	19.5535	Kg		Output-3 from fermentation stage	20.1374	Kg
Ammonia	0.0006	Kg				
Cellulase	0.0025	Kg		***Emission to Air***		
Corn steep liquor	0.0664	Kg		Water	0.0165	Kg
Zymomonas Mobilis	0.0262	Kg		Ethanol	0.0148	Kg
				Carbondioxide	0.9434	Kg
Utilities				Oxygen	0.0010	Kg
Water	1.4637	Kg				
Energy						
Electricity	0.00002	KWh				

Table F3.4 List of inventory of Alternative-3 in recovery stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Output-3 from Fermentation Stage	20.1374	Kg		Ethanol 99.5 wt%	1.0000	Kg
Energy						
Electricity	0.0000	KWh		***Liquid waste***		
Steam	15.2001	Kg		Waste water	18.9901	Kg

Table F3.5 List of inventory of Alternative-3 in biogas and cogeneration stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Waste water	18.9901	Kg		Steam	3.6350	Kg
				Electricity	0.9629	KWh
				Emission to air		
				Nitrogen oxides	1.77E-04	Kg
				Carbon monoxide	5.66E-04	Kg
				Methane, biogenic	2.71E-04	Kg
				NMVOC	2.36E-05	Kg
				Dinitrogen monoxide	2.95E-05	Kg
				Sulfur dioxide	2.48E-04	Kg
				Platinum	8.25E-11	Kg
				Heat, waste	1.04E+01	MJ
				Used mineral oil, to waste inceneration	3.54E-04	Kg

F.4 Alternative-4

Table F4.1 List of inventory of Alternative-4 in Pretreatment stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Sulphuric acid	0.0037	Kg		Output-1 from Pretreatment Stage	12.8913	Kg
Utilities				***Emission to Air***		
Water	3.1466	Kg		Water	2.2874	Kg
				Furfural	0.0047	Kg
Energy						
Steam	12.7669	Kg				

Table F4.2 List of inventory of Alternative-4 in Neutralization stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Output-1 from Pretreatment Stage	12.8913	Kg		Output-2 from Neutralization Stage	19.6761	Kg
Sulphuric acid	0.0338	Kg				
Calcium hydroxide	0.0275	Kg		***Solid Waste***		
				Gypsum	0.0505	Kg
Utilities				Glucose	0.0002	Kg
Water	6.9338	Kg		Xylose	0.0019	Kg
				Arabinose	0.0001	Kg
Energy				Cellulose	0.1480	Kg
Electricity	0.0002	KWh		Hemicellulose	0.0086	Kg
				Arabinan	0.0007	Kg
				Mannan	0.0001	Kg

Table F4.3 List of inventory of Alternative-4 in Fermentation stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Output-2 from neutralization stage	19.6761	Kg		Output-3 from fermentation stage	20.2637	Kg
Ammonia	0.0006	Kg				
Cellulase	0.0025	Kg		***Emission to Air***		
Corn steep liquor	0.07	Kg		Water	0.0166	Kg
Zymomonas Mobilis	0.0263	Kg		Ethanol	0.0149	Kg
				Carbondioxide	0.9493	Kg
Utilities				Oxygen	0.0010	Kg
Water	1.4729	Kg				
Energy						
Electricity	0.00002	KWh				

Table F4.4 List of inventory of Alternative-4 in recovery stage

Input Inventory				Output Inventory		
Type	**Amount**	**Unit**		**Type**	**Amount**	**Unit**
Material				***Product***		
Output-3 from Fermentation Stage	20.2637	Kg		Ethanol 99.5 wt%	1.0000	Kg
Energy						
Electricity	0.0044	KWh		***Liquid waste***		
Steam	6.1671	Kg		Waste water	19.2382	Kg

Table F4.5 List of inventory of Alternative-4 in biogas and cogeneration stage

Input Inventory				Output Inventory		
Type	**Amount**	**Unit**		**Type**	**Amount**	**Unit**
Material				***Product***		
Waste water	19.2382	Kg		Steam	3.8040	Kg
				Electricity	1.0077	KWh
				Emission to air		
				Nitrogen oxides	1.82E-04	Kg
				Carbon monoxide	5.81E-04	Kg
				Methane, biogenic	2.78E-04	Kg
				NMVOC	2.42E-05	Kg
				Dinitrogen monoxide	3.03E-05	Kg
				Sulfur dioxide	2.54E-04	Kg
				Platinum	8.48E-11	Kg
				Heat, waste	1.07E+01	MJ
				Used mineral oil, to waste inceneration	3.63E-04	Kg

F.5 Alternative-5

Table F5.1 List of inventory of Alternative-5 in Pretreatment stage

Input Inventory				Output Inventory		
Type	**Amount**	**Unit**		**Type**	**Amount**	**Unit**
Material				***Product***		
Sulphuric acid	0.0037	Kg		Output-1 from Pretreatment Stage	12.8913	Kg
Utilities				***Emission to Air***		
Water	0.0000	Kg		Water	2.2874	Kg
				Furfural	0.0047	Kg
Energy						
Steam	12.3160	Kg				

Table F5.2 List of inventory of Alternative-5 in Neutralization stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Output-1 from Pretreatment Stage	12.8913	Kg		Output-2 from Neutralization Stage	19.6762	Kg
Sulphuric acid	0.0338	Kg				
Calcium hydroxide	0.0275	Kg		***Solid Waste***		
				Gypsum	0.0505	Kg
Utilities				Glucose	0.0002	Kg
Water	6.9338	Kg		Xylose	0.0019	Kg
				Arabinose	0.0001	Kg
Energy				Cellulose	0.1480	Kg
Electricity	0.0002	KWh		Hemicellulose	0.0086	Kg
				Arabinan	0.0007	Kg
				Mannan	0.0001	Kg

Table F5.3 List of inventory of Alternative-5 in Fermentation stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Output-2 from neutralization stage	19.6762	Kg		Output-3 from fermentation stage	20.2638	Kg
Ammonia	0.0006	Kg				
Cellulase	0.0025	Kg		***Emission to Air***		
Corn steep liquor	0.0668	Kg		Water	0.0166	Kg
Zymomonas Mobilis	0.0263	Kg		Ethanol	0.0149	Kg
				Carbondioxide	0.9493	Kg
Utilities				Oxygen	0.0010	Kg
Water	1.4729	Kg				
Energy						
Electricity	0.00002	KWh				

Table F5.4 List of inventory of Alternative-5 in recovery stage

Input Inventory				Output Inventory		
Type	Amount	Unit		Type	Amount	Unit
Material				***Product***		
Output-3 from Fermentation Stage	20.2638	Kg		Ethanol 99.5 wt%	1.0000	Kg
Energy						
Electricity	0.0044	KWh		***Liquid waste***		
Steam	3.5511	Kg		Waste water	19.2383	Kg

Table F5.5 List of inventory of Alternative-5 in biogas and cogeneration stage

Input Inventory				Output Inventory		
Type	**Amount**	**Unit**		**Type**	**Amount**	**Unit**
Material				***Product***		
Waste water	19.2383	Kg		Steam	3.6392	Kg
				Electricity	0.9640	KWh
				Emission to air		
				Nitrogen oxides	1.66E-04	Kg
				Carbon monoxide	5.32E-04	Kg
				Methane, biogenic	2.55E-04	Kg
				NMVOC	2.22E-05	Kg
				Dinitrogen monoxide	2.77E-05	Kg
				Sulfur dioxide	2.33E-04	Kg
				Platinum	7.76E-11	Kg
				Heat, waste	983.06%	MJ
				Used mineral oil, to waste inceneration	3.33E-04	Kg

Appendix G Life Cycle Assessment of New Design Alternatives

Table G1 Comparison of life cycle impact assessment between the base case and new design alternatives per one kilogram ethanol 99.5 wt%

Impact category	Unit	Base case	Alternative-1	Alternative-2	Alternative-3	Alternative-4	Alternative-5
Abiotic depletion	kg Sb eq	1.23E-04	1.21E-04	1.20E-04	1.28E-04	9.84E-05	8.95E-05
Acidification	kg SO2 eq	2.76E-03	2.74E-03	2.69E-03	2.91E-03	2.14E-03	1.89E-03
Eutrophication	kg PO4--- eq	4.44E-04	4.37E-04	4.27E-04	4.78E-04	2.96E-04	2.42E-04
Global warming	kg CO2 eq	6.33E-02	6.28E-02	6.17E-02	6.65E-02	4.97E-02	4.32E-02
Ozone layer depletion	kg CFC-11 eq	2.18E-09	2.16E-09	2.13E-09	2.30E-09	1.69E-09	1.52E-09
Human toxicity	kg 1,4-DB eq	3.12E-02	3.08E-02	3.03E-02	3.32E-02	2.28E-02	1.97E-02
Fresh water aquatic ecotox.	kg 1,4-DB eq	1.57E-03	1.57E-03	1.57E-03	1.59E-03	1.49E-03	1.42E-03
Marine aquatic ecotoxicity	kg 1,4-DB eq	2.69E+00	2.67E+00	2.66E+00	2.75E+00	2.44E+00	2.31E+00
Terrestrial ecotoxicity	kg 1,4-DB eq	7.42E-05	7.39E-05	7.37E-05	7.55E-05	6.89E-05	6.63E-05
Photochemical oxidation	kg C2H4	6.87E-03	6.85E-03	6.83E-03	6.95E-03	2.51E-02	2.49E-02
Energy resources	MJ LHV	5.44E-01	5.36E-01	5.27E-01	5.79E-01	3.95E-01	3.42E-01

Table G2 Comparison of life cycle impact assessment between the base case and new design alternatives per one megajoule ethanol 99.5 wt%

Impact category	Unit	Base case	Alternative-1	Alternative-2	Alternative-3	Alternative-4	Alternative-5
Abiotic depletion	kg Sb eq	4.63E-06	4.58E-06	4.53E-06	4.84E-06	3.71E-06	3.38E-06
Acidification	kg SO2 eq	1.04E-04	1.03E-04	1.02E-04	1.10E-04	8.08E-05	7.13E-05
Eutrophication	kg PO4--- eq	1.67E-05	1.65E-05	1.61E-05	1.80E-05	1.12E-05	9.15E-06
Global warming	kg CO2 eq	2.39E-03	2.37E-03	2.33E-03	2.51E-03	1.87E-03	1.63E-03
Ozone layer depletion	kg CFC-11 eq	8.23E-11	8.14E-11	8.03E-11	8.66E-11	6.39E-11	5.72E-11
Human toxicity	kg 1,4-DB eq	1.18E-03	1.16E-03	1.14E-03	1.25E-03	8.60E-04	7.44E-04
Fresh water aquatic ecotox.	kg 1,4-DB eq	5.93E-05	5.92E-05	5.91E-05	6.01E-05	5.64E-05	5.37E-05
Marine aquatic ecotoxicity	kg 1,4-DB eq	1.01E-01	1.01E-01	1.00E-01	1.04E-01	9.21E-02	8.72E-02
Terrestrial ecotoxicity	kg 1,4-DB eq	2.80E-06	2.79E-06	2.78E-06	2.85E-06	2.60E-06	2.50E-06
Photochemical oxidation	kg C2H4	2.59E-04	2.59E-04	2.58E-04	2.62E-04	9.46E-04	9.41E-04
Energy resources	MJ LHV	2.05E-02	2.02E-02	1.99E-02	2.18E-02	1.49E-02	1.29E-02

CURRICULUM VITAE

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- Completing Process simulation using PRO/II and sustainability analysis using SustainPro from the Computer Aided Process Engineering System Center (CAPEC), Department of Chemical and Biochemical Engineering, Technical University of Denmark, Lyngby, Denmark, 2009