Electronic Supplementary Material (ESI) for RSC Advances

FUELS AND PLASTICS FROM LIGNOCELLULOSIC BIOMASS VIA THE FURAN PATHWAY; A TECHNICAL ANALYSIS

A.J.J.E Eerhart [*a], W.J.J. Huijgen [b], R.J.H. Grisel [b], J.C. van der Waal [c],
E. de Jong [c], A. de Sousa Dias [c], A.P.C. Faaij [a], M.K. Patel [a]

a: Department of Innovation, Environmental and Energy Sciences
Copernicus Institute of Sustainable Development, Utrecht University
Heidelberglaan 2, 3584 CS, Utrecht, the Netherlands
Tel: +31 30 253 5144; Fax: +31 30 253 7601
[*] corresponding author: a.eerhart@uu.nl

b: Biomass & Energy Efficiency, Energy Research Centre of the Netherlands (ECN)
Westerduinweg 3, 1755 LE, Petten, the Netherlands

c: Avantium Chemicals B.V.
Zekeringstraat 29, 1014 BV, Amsterdam, the Netherlands

Electronic Supplementary Material (ESI) for RSC Advances

ELECTRONIC SUPPLEMENTARY INFORMATION

E.S.I., part I: modeling assumptions for the ASPEN Plus models

E.S.I., part II: individual flowsheets of hierarchies

E.S.I., part III: flowsheet and stream tables of case I, II and III

E.S.I., PART I: MODELING ASSUMPTIONS FOR THE ASPEN PLUS MODELS

The following table shows the components used in the ASPEN Plus models. Wherever possible, native ASPEN Plus components were used. However, several components were not available in the native ASPEN Plus database and were introduced into the simulation file, either through estimation of properties using the NIST ThermoDynamic Engine or via the NREL user-based database.

Component	Type	Reference	Notes
Acetic acid	Mixed	Native ASPEN Plus component	
Formaldehyde	Mixed	Native ASPEN Plus component	
Ash (chlorine, soluble)	Mixed	Native ASPEN Plus component	
Carbon dioxide	Mixed	Native ASPEN Plus component	
Dimethyl ether	Mixed	Native ASPEN Plus component	
Ethanol	Mixed	Native ASPEN Plus component	
Formic acid	Mixed	Native ASPEN Plus component	
2,5-dicarboxylic acid (FDCA)	Mixed	Native ASPEN Plus component	
furfuryl ethyl ether (FEE)	Mixed	Properties for FEE were estimated using the NIST TDE	1
Fructose	Mixed	Duplicate of glucose	2
Furfuryl alcohol	Mixed	Native ASPEN Plus component	
Furfural	Mixed	Native ASPEN Plus component	
Glucose	Mixed	Native ASPEN Plus component (dextrose)	3
Hydrogen	Mixed	Native ASPEN Plus component	
Sulfuric acid	Mixed	Native ASPEN Plus component	
5-hydroxymethyl furfural (HMF)	Mixed	NREL inhouse database	4
Ash (potassium, soluble)	Mixed	Native ASPEN Plus component	
Levulinic acid	Mixed	Native ASPEN Plus component	
Lignin (soluble)	Mixed	NREL inhouse database	4
Methanol	Mixed	Native ASPEN Plus component	
Methylal	Mixed	Native ASPEN Plus component	
Methyl formate	Mixed	Native ASPEN Plus component	
Methyl levulinate	Mixed	Properties for FEE were estimated using the NIST TDE	1
5-methoxymethyl furfural (MMF)	Mixed	Properties for FEE were estimated using the NIST TDE	1
Nitrogen	Mixed	Native ASPEN Plus component	
Oxygen	Mixed	Native ASPEN Plus component	
Rest (soluble)	Mixed	Native ASPEN Plus component (citric acid)	5
Water	Mixed	Native ASPEN Plus component	
Xylose	Mixed	Native ASPEN Plus component	
Cellulose	Solid	Native ASPEN Plus component	6
Humins (glucose)	Solid	Native ASPEN Plus component (dibenzofuran)	7
Humins (xylose)	Solid	Native ASPEN Plus component (dibenzofuran)	7
Ash (potassium chloride)	Solid	Native ASPEN Plus component	
Lignin (insoluble)	Solid	NREL inhouse database	
Rest (insoluble)	Solid	Native ASPEN Plus component (citric acid)	
Ash (insoluble)	Solid	Native ASPEN Plus component (silicon dioxide)	
Xylan	Solid	Native ASPEN Plus component	8

1. Based on the molecular weight, structure and boiling point, the NIST ThermoDynamic Engine database is accessed. If the component is listed, important properties, such as the heat of formation, are imported into the model. If not, the TDE routines in ASPEN Plus will estimate these properties.
2. Glucose is used to represent fructose, with a modification to the molar structure.
3. Dextrose is used to represent glucose.
4. The NREL inhouse database was created to introduce components not available in the ASPEN Plus native database (http://www.nrel.gov/extranet/biorefinery/aspen_models/).
5. Experimental composition analysis of wheat straw accounted for 93.8%[28]. By looking at the CHO ratio, the unknown fraction has a similar composition as citric acid and is therefore modeled as such.
6. Native ASPEN Plus component, with back calculated heat of formation.
7. After the furan conversion, the remainder of the mass balance was calculated. By looking at the CHO ratio, the fraction has a similar composition is dibenzofuran.
8. Native ASPEN Plus component, with back calculated heat of formation

E.S.I., PART II: INDIVIDUAL FLOWSHEETS OF HIERARCHIES

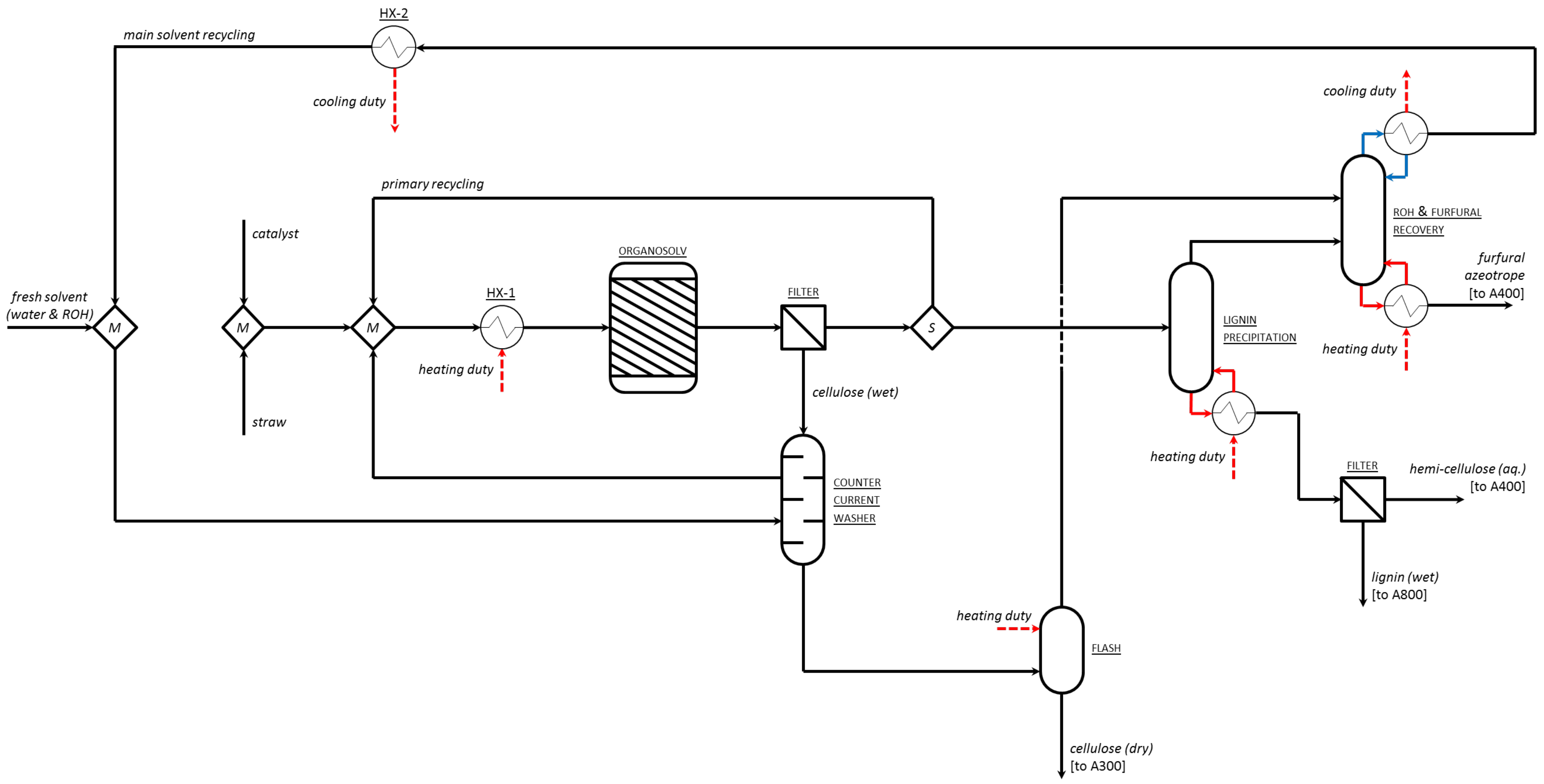

Figure 1: case I and II; flowsheet hierarchy A200

CASE I			CASE II	
Organosolv reactor (case I, ethanol)			**Organosolv reactor (case II, methanol)**	
Temperature = 200°C Vapor fraction = 0 L/S ratio = 5/1 (w/w)			Temperature = 200°C Vapor fraction = 0 L/S ratio = 5/1	
Reactions, occurring in series: Lignin (solid) → lignin (mixed) Xylan (solid) + water → xylose Xylose → furfural + 3 water KCL (solid) → K+ + Cl- Rest-saq (solid) → rest-aq (mixed)	Fractional conversion: 0.8 0.8 0.375 1.0 1.0		Reactions, occurring in series: Lignin (solid) → lignin (mixed) Xylan (solid) + water → xylose Xylose → furfural + 3 water KCL (solid) → K+ + Cl- Rest-saq (solid) → rest-aq (mixed)	Fractional conversion: 0.6 0.8 0.375 1.0 1.0
Counter current washer			**Counter current washer**	
2-stage atmospheric washer			2-stage atmospheric washer	
Flash			**Flash**	
Temperature = 175°C Pressure = 1 bar			Temperature = 175°C Pressure = 1	
Lignin precipitation column (no condenser)			**Lignin precipitation column (no condenser)**	
Stages = 20 Pressure = 1 bar Distillate rate = 96068 kg/hr Design spec. = 10 mass% recovery furfural in bottom stream			Stages = 20 Pressure = 1 bar Distillate rate = 98500 kg/hr Design spec. = 10 mass% recovery furfural in bottom stream	
ROH & furfural recovery column (partial vapor condenser)			**ROH & furfural recovery column (partial vapor condenser)**	
Stages = 20 Pressure = 1 bar Distillate rate = 200,000 kg/hr Design spec. = 99.8 mass% recovery of ethanol in top stream			Stages = 20 Pressure = 1 bar Distillate rate = 173,500 kg/hr Design spec. = 99.8 mass% recovery of methanol in top stream	
HX-1			**HX-1**	
Temperature in = 82°C Temperature out = 200°C			Temperature in = 77°C Temperature out = 200°C	
HX-2			**HX-2**	
Temperature in = 79°C Temperature out = 20°C			Temperature in = 73°C Temperature out = 20°C	

Electronic Supplementary Material (ESI) for RSC Advances
This journal is © The Royal Society of Chemistry 2014

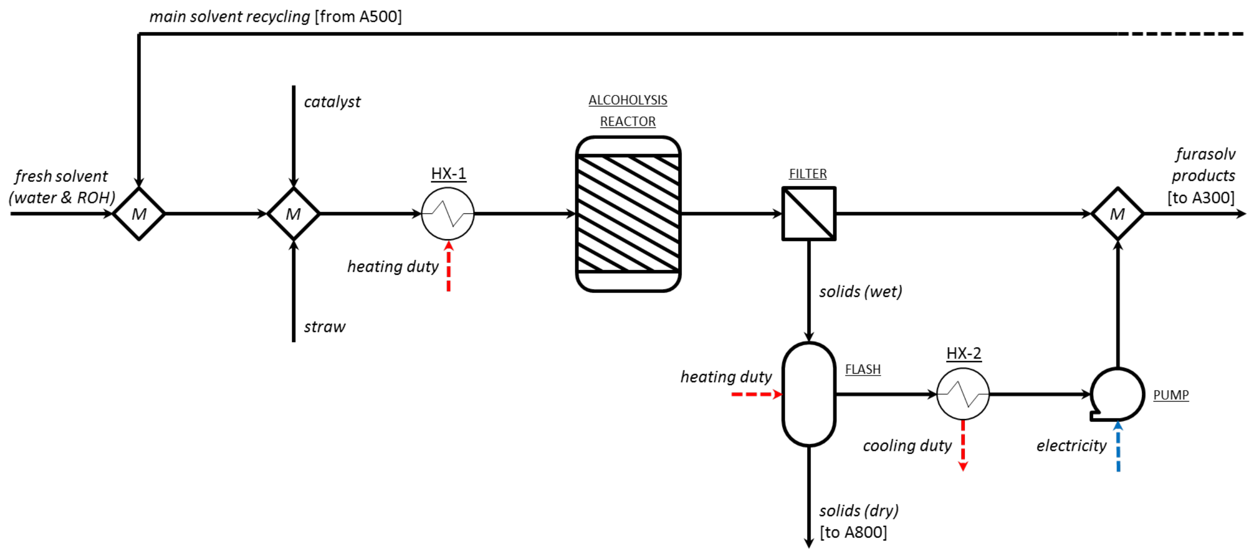

Figure 2: case III; flowsheet hierarchy A200

CASE III	
Alcoholysis reactor (case III, methanol)	
Temperature = 200°C Vapor fraction = 0 L/S ratio = 4/1	
Reactions, occurring in series:	Fractional conversion:
Lignin (solid) → lignin (mixed)	0.7
Rest-saq (solid → rest-aq (mixed)	1.0
Cellulose (solid) + water → glucose	0.94
Xylan (solid) + water → xylose	1.0
Glucose → HMF + 3 water	0.24
Xylose → furfural + 3 water	0.413
HMF + methanol → MMF + water	0.81696
MMF + 2 water → ML + formic acid	0.83606
9 glucose → 4 glucose-humins + 38 water + 6 CO2	0.38966
27 xylose → 10 xylose-humins + 95 water + 15 CO2	0.8756
KCL (solid) → K+ + Cl-	1.0
2 methanol → DME + water	0.1
Formic acid + methanol → MF + water	1.0
Flash	
Temperature = 170°C Pressure = 1	
HX-1	
Temperature in = 21°C Temperature out = 200°C Vapor fraction = 0	
HX-2	
Temperature in = 170°C Temperature out = 24°C Vapor fraction = 0	
Pump	
Outlet pressure = 40 bar (vapor phase = 0)	

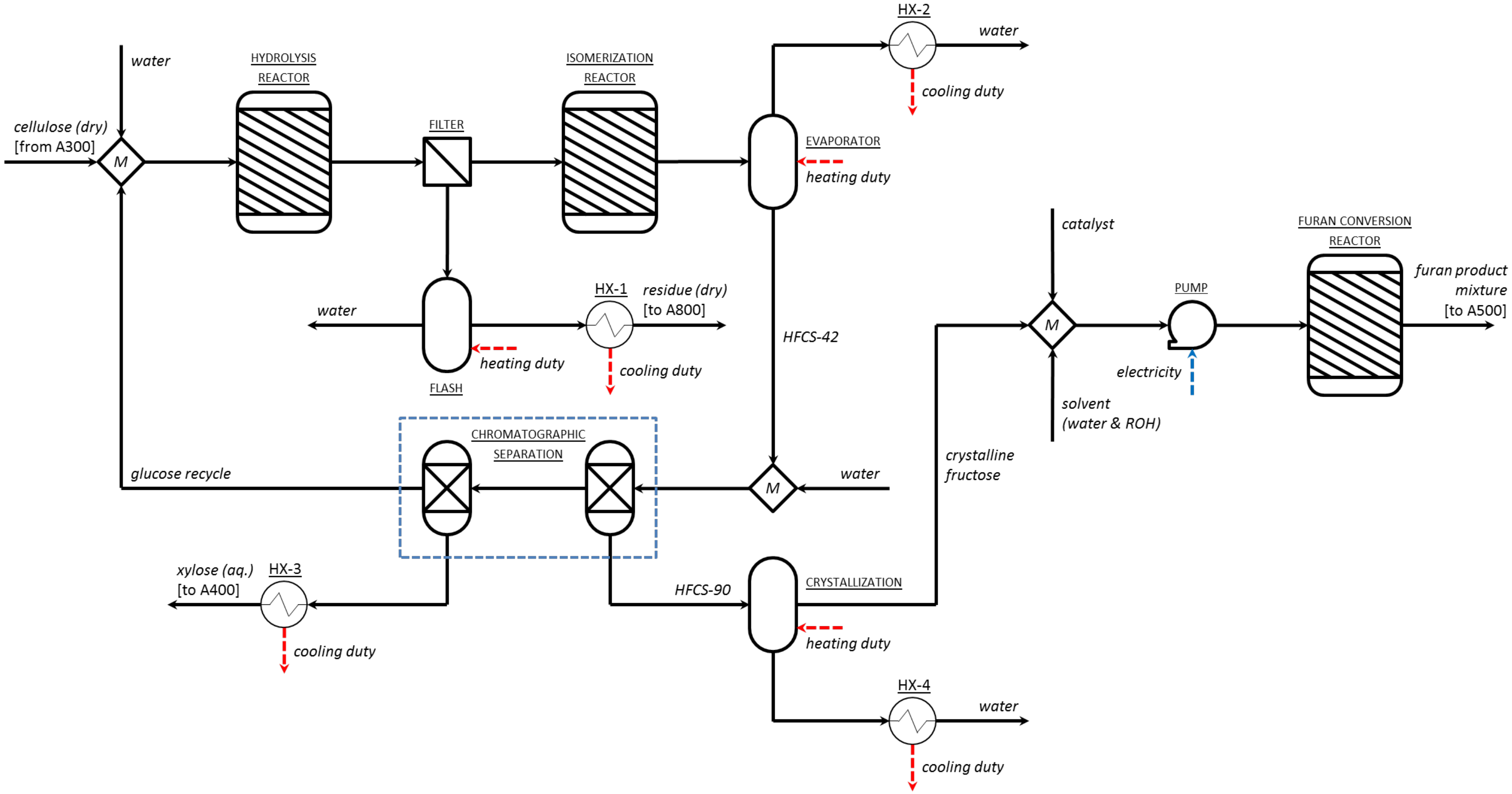

Figure 3: case I; flowsheet hierarchy A300

<table>
<tr><th colspan="5">CASE I</th></tr>
<tr><td colspan="2">Hydrolysis reactor</td><td></td><td colspan="2">Furan conversion reactor</td></tr>
<tr><td colspan="2">Temperature = 50°C
Pressure = 1 bar</td><td></td><td colspan="2">Temperature = 200°C
Pressure = 50 bar</td></tr>
<tr><td>Reactions:
Xylan (solid) + water → xylose
Cellulose (solid) + water → glucose</td><td>Fractional conversion:
1.00
0.95</td><td></td><td>Reactions, occurring in series:
Fructose → HMF + 3 water
HMF + methanol → MMF + water
HMF + 2 water → levulinic-acid + formic-acid
Levulinic acid + methanol → ML + water
Formic acid + methanol → MF + water
Fructose → formaldehyde + 3 water + furfural
Formaldehyde + 2 methanol → methylal + water
Fructose → 0.44 glucose-humins + 4.22 water + 0.66 CO2
Xylose → furfural + 3 water
Xylose → 0.37 xylose-humins + 3.52 water + 0.56 CO2</td><td>Molar conversion (kmol/hr):
105
77
13

12
2.5
4

1.0 (fractional conversion)

44

0.8 (fractional conversion)
1.0 (fractional conversion)</td></tr>
<tr><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td colspan="2">Isomerization reactor</td><td></td><td colspan="2">Crystallization</td></tr>
<tr><td colspan="2">Temperature = 50°C
Pressure = 1 bar</td><td></td><td colspan="2">Temperature = 105°C
Pressure = 1 bar</td></tr>
<tr><td>Reaction:
Glucose → fructose</td><td>Fractional conversion:
0.42</td><td></td><td colspan="2"></td></tr>
<tr><td colspan="2"></td><td></td><td colspan="2"></td></tr>
<tr><td colspan="2">Evaporator</td><td></td><td colspan="2">Pump</td></tr>
<tr><td colspan="2">Temperature = 105°C
Pressure = 1 bar
Design spec. = 60% of water in isomerization reactor effluent removed from sugar stream by controlling the temperature of evaporation</td><td></td><td colspan="2">Outlet pressure = 50 bar</td></tr>
</table>

Chromatographic separation		**Flash**
Temperature = 65°C Pressure = 1 bar Design spec. 1 = water added to HFCS-42 is equal to total volume of HFCS-42, multiplied by 2.68, based on reference 59 (Purolite, 2007) Design spec. 2 = 90% of fructose and 4.5% of glucose to HFCS-90, including 40% of water Design spec. 3 = 90% of xylose and 4.5% of glucose to xylose (aq.) stream, including 40% of water		Temperature = 175°C Pressure = 1 bar
HX-1		**HX-3**
Temperature in = 175°C Temperature out = 20°C		Temperature in = 65°C Temperature out = 20°C
HX-2		**HX-4**
Temperature in = 105°C Temperature out = 20°C		Temperature in = 105°C Temperature out = 20°C

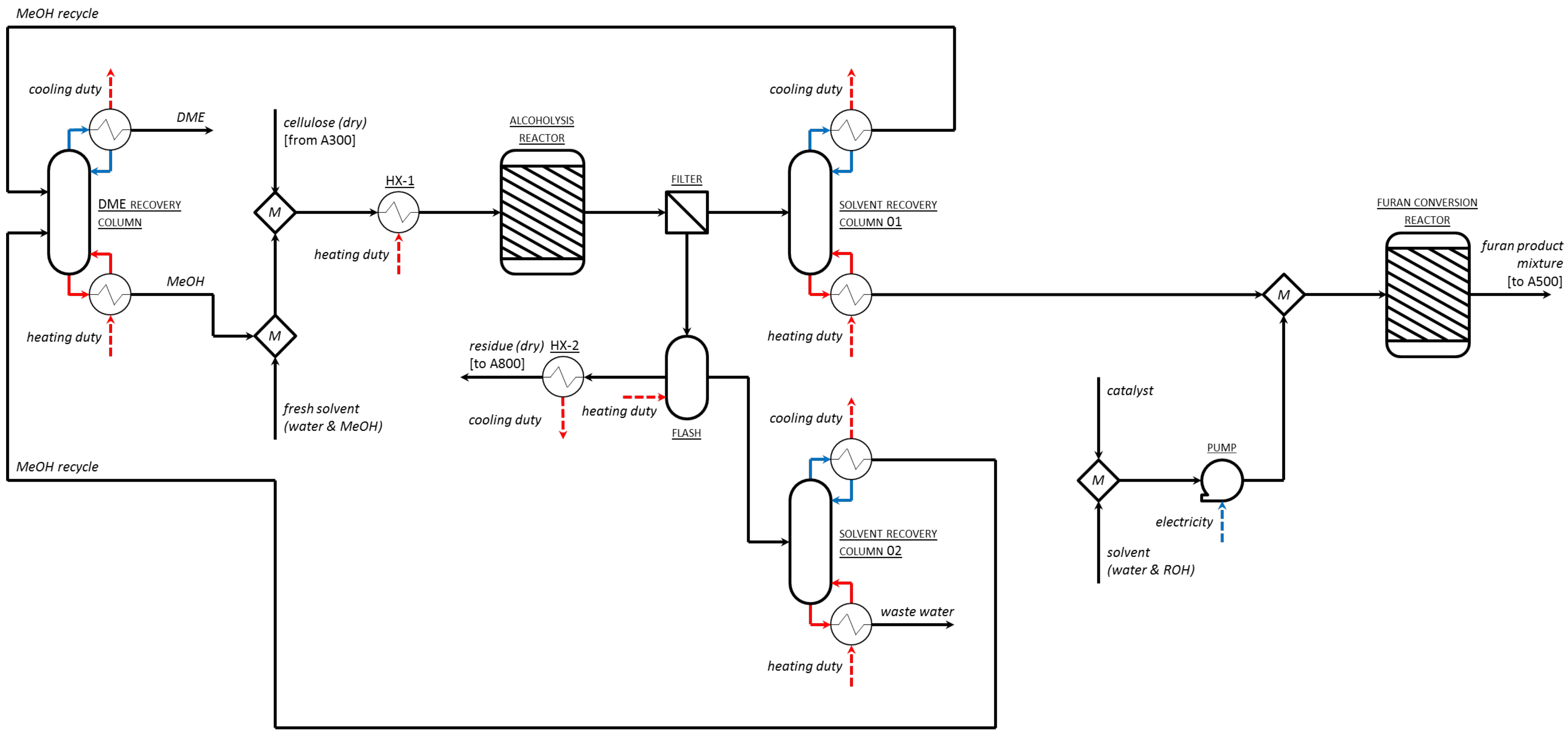

Figure 4: case II; flowsheet hierarchy A300

CASE II

Alcoholysis reactor			**Furan conversion reactor**	
Temperature = 200°C Vapor fraction = 0 Design spec. = L/S ratio = 4, by adding fresh solvent			Temperature = 200°C Pressure = 50 bar	
Reactions, occurring in series:	Fractional conversion:		Reactions, occurring in series:	Molar conversion (kmol/hr):
Cellulose (solid) + water → glucose	0.55		Glucose → HMF + 3 water	105
Cellulose (solid) → HMF + 2 water	0.1		HMF + methanol → MMF + water	77
Cellulose (solid) + methanol → MMF + 3 water	0.05		HMF + 2 water → levulinic-acid + formic-acid	13
			Levulinic acid + methanol → ML + water	12
Cellulose (solid) → levulinic acid + formic acid	0.01		Formic acid + methanol → MF + water	2.5
			Glucose → formaldehyde + 3 water + furfural	4
Cellulose (solid) + methanol → ML + formic acid + water	0.1		Formaldehyde + 2 methanol → methylal + water	1.0 (fractional conversion)
			Fructose → 0.44 glucose-humins + 4.22 water + 0.66 CO2	44
Xylan (solid) + water → xylose	0.02			
Xylan (solid) → furfural + 2 water	0.5		Xylose → furfural + 3 water	0.8 (fractional conversion)
2 methanol → DME + water	0.1		Xylose → 0.37 xylose-humins + 3.52 water + 0.56 CO2	1.0 (fractional conversion)
Flash			**Pump**	
Temperature = 175°C Pressure = 1 bar			Outlet pressure = 50 bar	
HX-1			**HX-2**	
Temperature in = 20°C Temperature out = 200°C Vapor fraction = 0			Temperature in = 175°C Temperature out = 20°C	
Solvent recovery column 1 (partial vapor condenser)			**Solvent recovery column 2 (partial vapor condenser)**	
Stages = 20 Pressure = 1 Distillate rate = 35000 kg/hr Design spec. = 99.5 mass% recovery of methanol in top stream			Stages = 20 Pressure = 1 bar Distillate rate = 115000 kg/hr Design spec. = 80 mass% recovery of water in top stream	
DME recovery column (partial vapor condenser)				
Stages = 20 Pressure = 1 bar Distillate rate = 30000 kg/hr Design spec. = 99.5 mass% recovery of methanol in bottom stream				

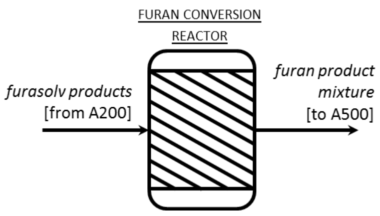

Figure 5: case III; flowsheet hierarchy A300

CASE III	
Furan conversion reactor	
Temperature = 200°C Vapor fraction = 0	
Reactions, occurring in series:	Fractional conversion:
Glucose → HMF + 3 water	0.414
HMF + methanol → MMF + water	0.97
MMF + 2 water → ML + formic acid	0.625
27 xylose → 10 xylose-humins + 95 water + 15 CO_2	1.0
Formic acid + methanol → MF + water	1.0
9 glucose → 4 glucose-humins + 38 water + 6 CO_2	0.68

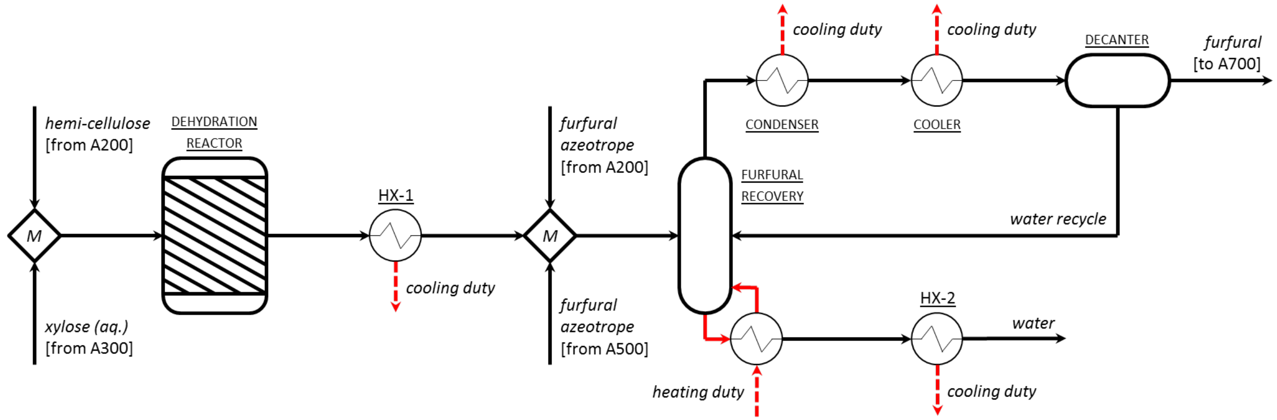

Figure 6: case I; flowsheet hierarchy A400

CASE I			
Dehydration reactor			**Furfural recovery column (no condenser)**
Temperature = 150°C Vapor fraction = 0 Pressure = 4.8 bar			Stages = 20 Pressure = 1 Distillate rate = 50000 kg/hr
Reaction: Xylose → furfural + 3 water	Fractional conversion: 0.5		
HX-1			**HX-2**
Temperature in = 150°C Temperature out = 97°C Pressure = 1 bar			Temperature in = 100°C Temperature out = 20°C Pressure = 1 bar
Condenser			**Cooler**
Temperature in = 98°C Temperature out = 96°C Vapor fraction = 0 (1 bar pressure)			Temperature in = 96°C Temperature out = 0°C Pressure = 1 bar
Decanter			
2^{nd} liquid phase = water			

Electronic Supplementary Material (ESI) for RSC Advances
This journal is © The Royal Society of Chemistry 2014

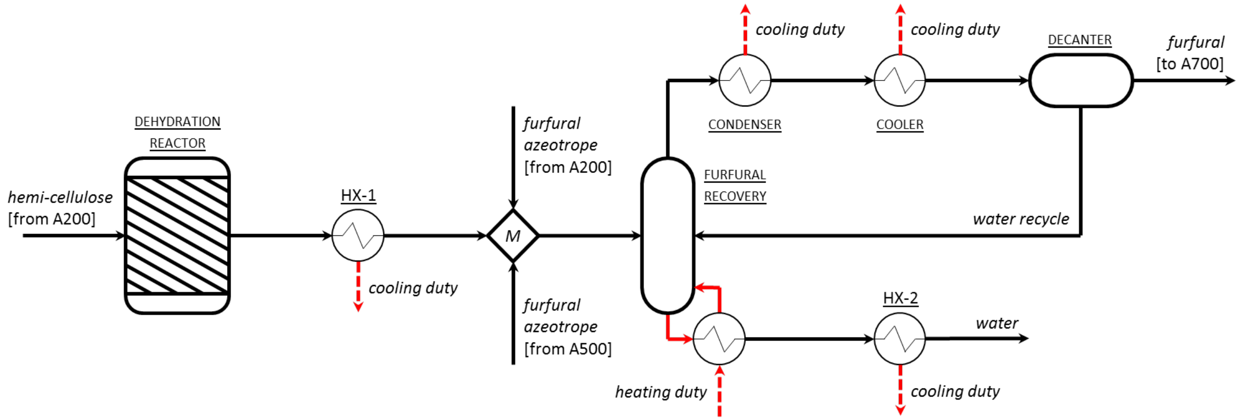

Figure 7: case II; flowsheet hierarchy A400

CASE II			
Dehydration reactor			**Furfural recovery column (no condenser)**
Temperature = 150°C Vapor fraction = 0 Pressure = 4.8 bar			Stages = 20 Pressure = 1 Distillate rate = 50000 kg/hr
Reaction: Xylose → furfural + 3 water	Fractional conversion: 0.5		
HX-1			**HX-2**
Temperature in = 150°C Temperature out = 97°C Pressure = 1 bar			Temperature in = 100°C Temperature out = 20°C Pressure = 1 bar
Condenser			**Cooler**
Temperature in = 98°C Temperature out = 96°C Vapor fraction = 0 (1 bar pressure)			Temperature in = 96°C Temperature out = 0°C Pressure = 1 bar
Decanter			
2^{nd} liquid phase = water			

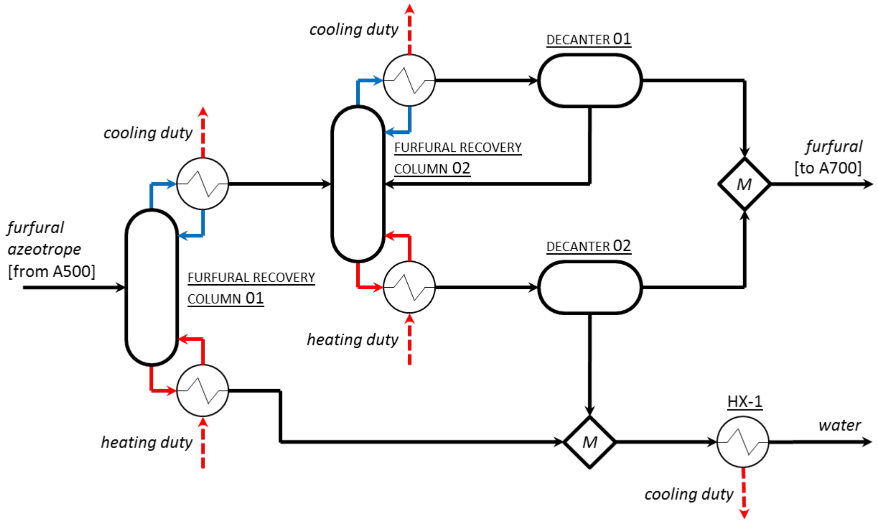

Figure 8: case III; flowsheet hierarchy A400

CASE III		
Primary furfural recovery column (total condenser)		**Secondary furfural recovery column (total condenser)**
Stages = 30 Pressure = 1 Distillate rate = 12000 kg/hr		Stages = 30 Pressure = 1 Distillate rate = 10000 kg/hr
Decanter 1		**Decanter 2**
2nd liquid phase = water		2nd liquid phase = water
HX-1		
Temperature in = 97°C Temperature out = 20°C Pressure = 1 bar		

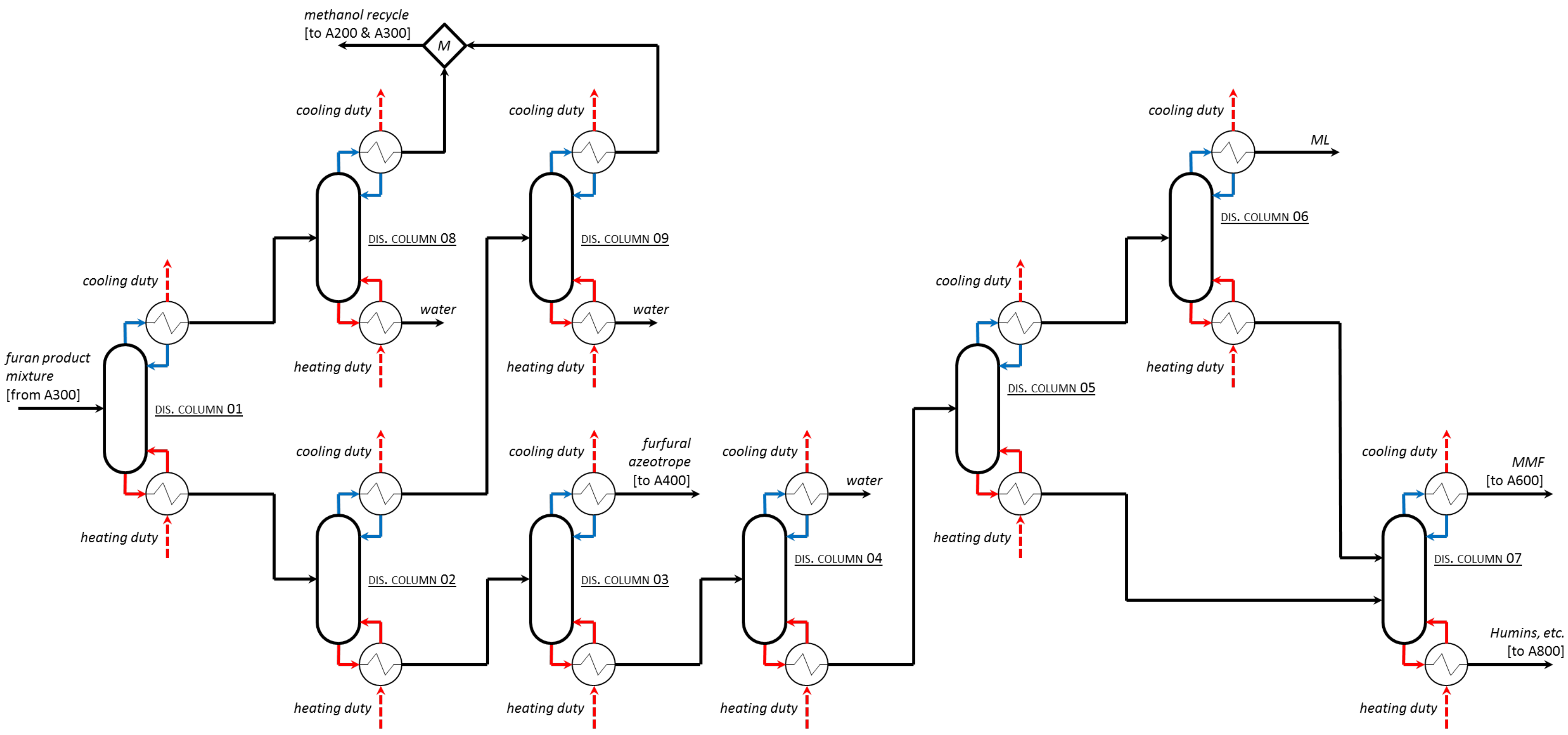

Figure 9: case I and II; flowsheet hierarchy A500

CASE I		CASE II
Distillation column 1 (partial-vapor condenser)		**Distillation column 1 (partial-vapor condenser)**
Stages = 30 Pressure = 25 bar Distillate rate = 31000 kg/hr Design spec. = 50 mass% recovery methanol in top stream		Stages = 30 Pressure = 25 bar Distillate rate = 20500 kg/hr Design spec. = 50 mass% recovery methanol in top stream
Distillation column 2 (partial-vapor condenser)		**Distillation column 2 (partial-vapor condenser)**
Stages = 30 Pressure = 12 bar Distillate rate = 29500 kg/hr Design spec. = 99.9 mass% recovery methanol in top stream		Stages = 30 Pressure = 12 bar Distillate rate = 19500 kg/hr Design spec. = 99.9 mass% recovery methanol in top stream
Distillation column 3 (partial-vapor condenser)		**Distillation column 3 (partial-vapor condenser)**
Stages = 20 Pressure = 1 bar Distillate rate = 6500 kg/hr Design spec. = 99.9 mass% recovery furfural in top stream		Stages = 20 Pressure = 1 bar Distillate rate = 4000 kg/hr Design spec. = 99.9 mass% recovery furfural in top stream
Distillation column 4 (total condenser)		**Distillation column 4 (total condenser)**
Stages = 20 Pressure = 0.2 bar Distillate rate = 2600 kg/hr Design spec. = 99.0 mass% recovery water in top stream		Stages = 20 Pressure = 0.2 bar Distillate rate = 3200 kg/hr Design spec. = 99.0 mass% recovery water in top stream
Distillation column 5 (total condenser)		**Distillation column 5 (total condenser)**
Stages = 20 Pressure = 0.15 bar Distillate rate = 2000 kg/hr Design spec. = 99.0 mass% recovery ML in top stream		Stages = 20 Pressure = 0.15 bar Distillate rate = 1600 kg/hr Design spec. = 99.0 mass% recovery ML in top stream
Distillation column 6 (total condenser)		**Distillation column 6 (total condenser)**
Stages = 20 Pressure = 0.15 bar Distillate rate = 1200 kg/hr Design spec. = 99.9 mass% recovery MMF in bottom stream		Stages = 20 Pressure = 0.15 bar Distillate rate = 1400 kg/hr Design spec. = 99.9 mass% recovery MMF in bottom stream

Distillation column 7 (total condenser)		**Distillation column 7 (total condenser)**
Stages = 20 Pressure = 0.015 bar Distillate rate = 8100 kg/hr Design spec. = 99.0 mass% recovery MMF in top stream		Stages = 20 Pressure = 0.015 bar Distillate rate = 5250 kg/hr Design spec. = 99.0 mass% recovery MMF in top stream
Distillation column 8 (partial-vapor condenser)		**Distillation column 8 (partial-vapor condenser)**
Stages = 20 Pressure = 1 bar Distillate rate = 28200 kg/hr Design spec. = 99.9 mass% recovery methanol in top stream		Stages = 20 Pressure = 1 bar Distillate rate = 19000 kg/hr Design spec. = 99.9 mass% recovery methanol in top stream
Distillation column 9 (partial-vapor condenser)		**Distillation column 9 (partial-vapor condenser)**
Stages = 20 Pressure = 1 bar Distillate rate = 26800 kg/hr Design spec. = 99.9 mass% recovery methanol in top stream		Stages = 20 Pressure = 1 bar Distillate rate = 18500 kg/hr Design spec. = 99.9 mass% recovery methanol in top stream

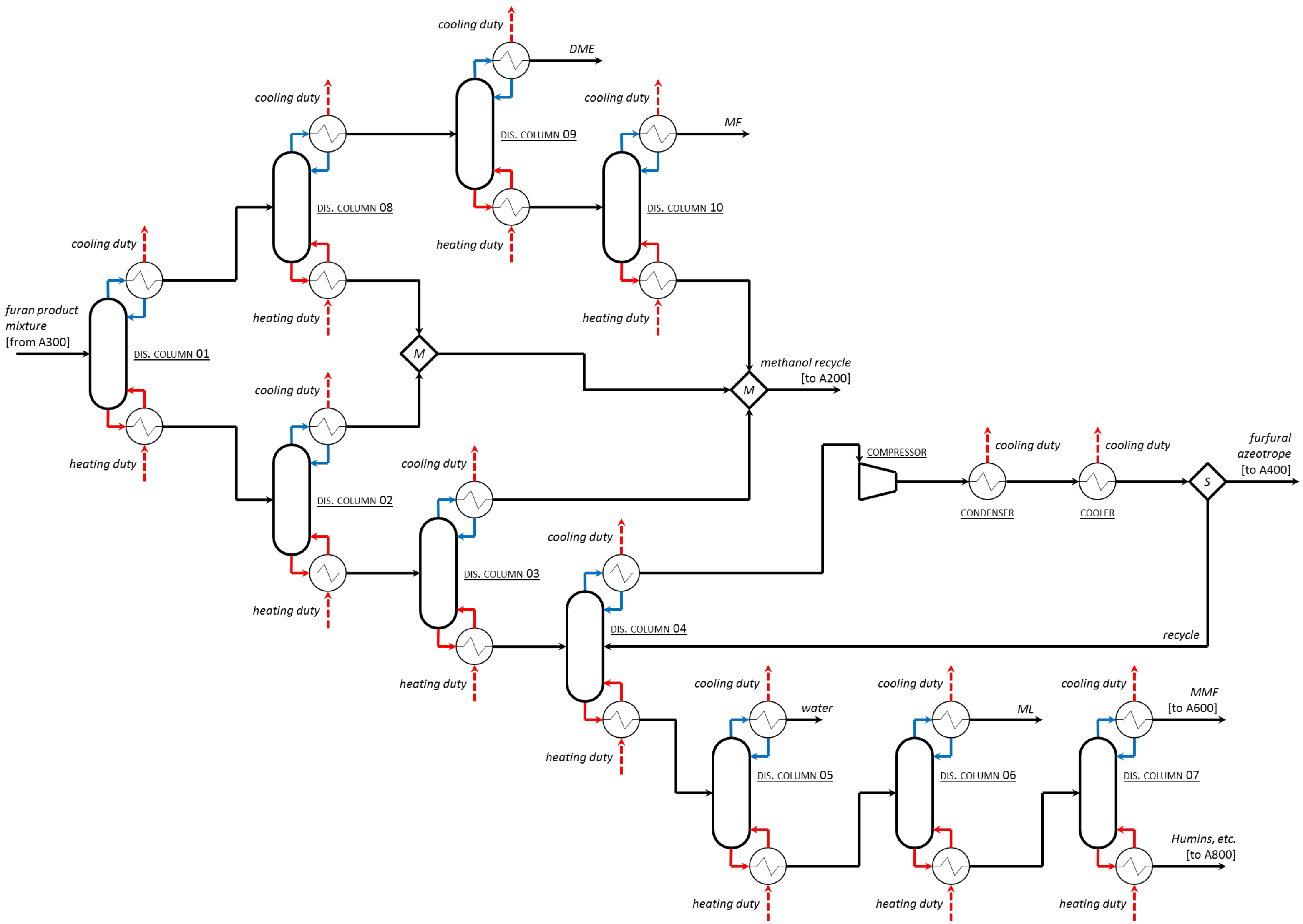

Figure 10: case III; flowsheet hierarchy A500

CASE III		
Distillation column 1 (total condenser)		**Distillation column 6 (total condenser)**
Stages = 30 Pressure = 30 bar Distillate rate = 141000 kg/hr | reflux ratio = 0.81		Stages = 27 Pressure = 0.15 bar Distillate rate = 7000 kg/hr Design spec. = 99.9 mass% recovery ML in top stream
Distillation column 2 (total condenser)		**Distillation column 7 (total condenser)**
Stages = 30 Pressure = 10 bar Distillate rate = 99000 kg/hr | reflux ratio = 0.6		Stages = 15 Pressure = 0.015 bar Distillate rate = 2200 kg/hr | reflux ratio = 10
Distillation column 3 (total condenser)		**Distillation column 8 (total condenser)**
Stages = 30 Pressure = 2 bar Distillate rate = 68000 kg/hr | reflux ratio = 1.4		Stages = 20 Pressure = 12 bar Distillate rate = 81250 kg/hr | reflux ratio = 0.22
Distillation column 4 (no condenser)		**Distillation column 9 (total condenser)**
Stages = 30 Pressure = 1 bar Distillate rate = 28500 kg/hr		Stages = 20 Pressure = 15 bar Distillate rate = 25500 kg/hr Design spec. = 99.9 mass% recovery DME in top stream
Distillation column 5 (total condenser)		**Distillation column 10 (total condenser)**
Stages = 10 Pressure = 0.2 bar Distillate rate = 14000 kg/hr Design spec. = 99.9 mass% recovery water in top stream		Stages = 20 Pressure = 15 bar Distillate rate = 3200 kg/hr Design spec. = 99.9 mass% recovery MF in top stream
Compressor		**Cooler**
Outlet pressure = 1.4 bar		Temperature in = 137°C Temperature out = 106°C Pressure = 1.4 bar
		Condenser
		Temperature in = 106°C Temperature out = 0°C Pressure = 1.4 bar

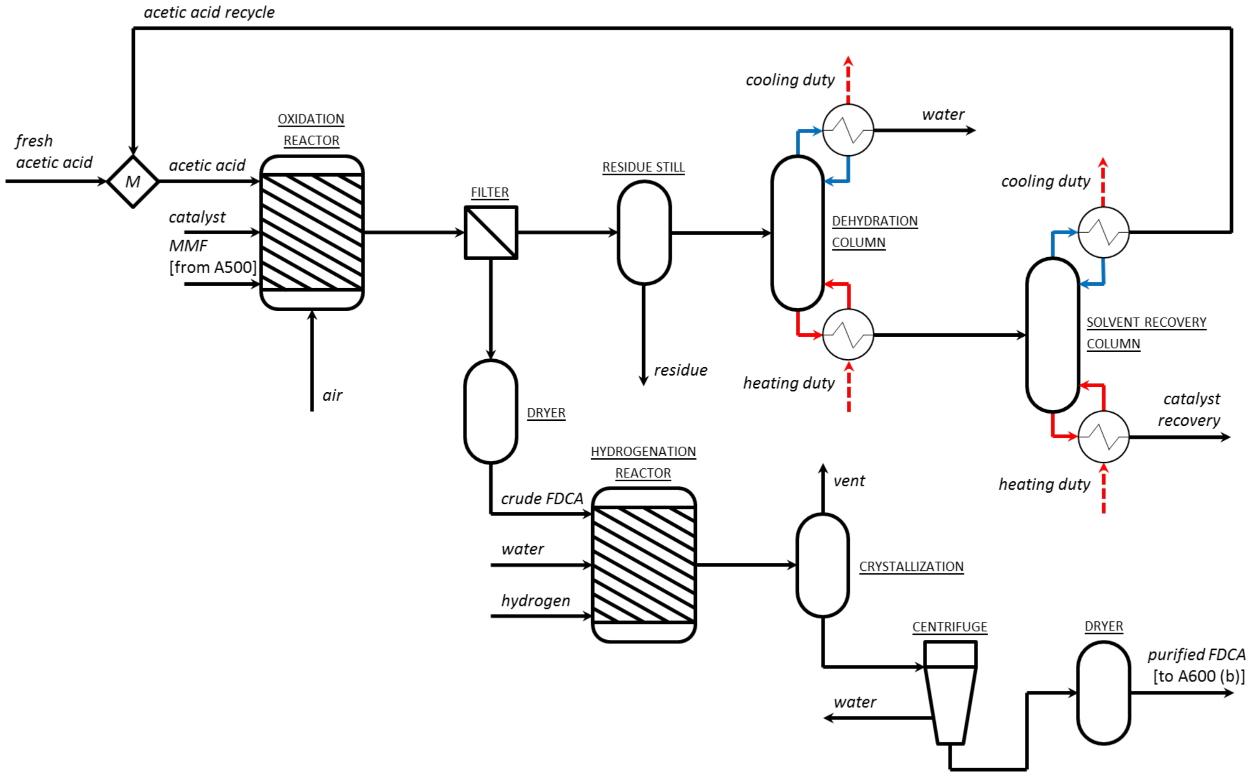

Figure 11: case I, II and III; flowsheet hierarchy A600 (a)

ALL CASES	
Oxidation reactor	
Temperature = 175°C Pressure = 20 bar	
Reactions, occurring in series: MMF + 1.5 O2 → FDCA + methanol	Fractional conversion: 0.95
Primary crystallizer	
Temperature = 180°C Pressure = 6 bar	
Hydrogenation reactor	
Temperature = 250°C Pressure = 40 bar	
Dehydration column	
Stages = 40 Pressure = 1 bar Distillate rate = 14000 kg/hr Design spec. = 99.9 mass% recovery water in top stream	
Solvent recovery column	
Stages = 20 Pressure = 1 bar Design spec. = product purity 99.5 mass%	

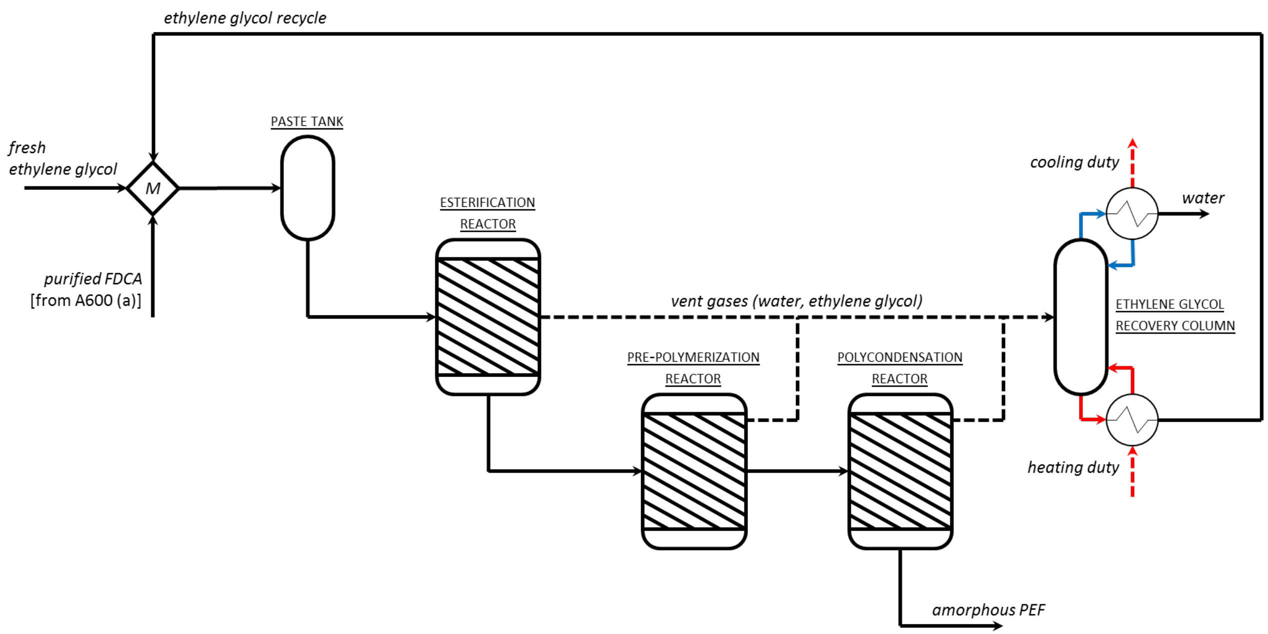

Figure 12: case I, II and III; flowsheet hierarchy A600 (b)

ALL CASES
Esterification reactor
Temperature = 260°C Pressure = 8 bar
Pre-polymerization reactor
Temperature = 260°C Pressure = 0.1 bar
Polycondensation reactor
Temperature = 280°C Pressure = 0.1 bar
Ethylene glycol recovery column
Not modeled

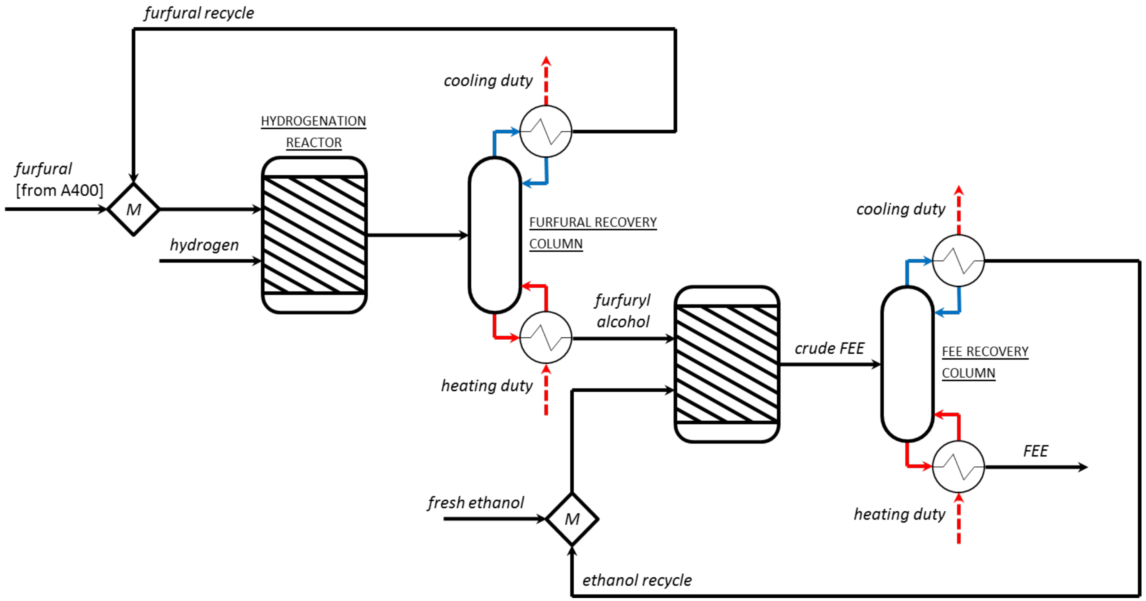

Figure 13: case I, II and III; flowsheet hierarchy A700

ALL CASES	
Hydrogenation reactor	
Temperature = 120°C Pressure = 1 bar	
Reactions, occurring in series: Furfural + H2 → furfuryl alcohol	Fractional conversion: 0.95
Furfural recovery column (partial-vapor condenser)	
Stages = 20 Pressure = 1 bar Distillate rate = 1000 kg/hr	
Etherification reactor	
Pressure = 1 bar Vapor fraction = 0	
FEE recovery column (partial-vapor condenser)	
Stages = 25 Pressure = 1 bar Distillate rate = 10000 kg/hr Design spec. = 99.0 mass% purity FEE in bottom stream	

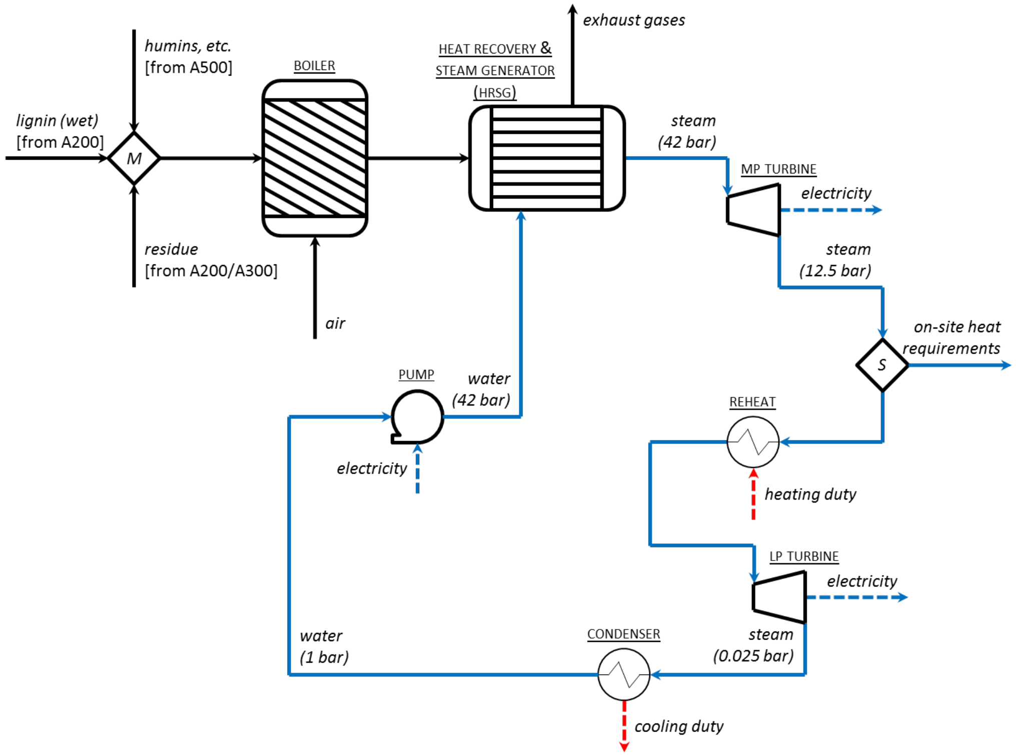

Figure 14: case I, II and III; flowsheet hierarchy A800 (note the water/steam cycle is marked in blue)

ALL CASES

Boiler

Temperature = 870°C
Pressure = 1 atm

Reactions, occurring in series:	Fractional conversion:
Ethanol + 3 O2 → 2 CO2 + 3 water	1.0
Fructose + 6 O2 → 6 CO2 + 6 water	1.0
Fufural + 5 O2 → 5 CO2 + 2 water	1.0
Glucose + 6 O2 → 6 CO2 + 6 water	1.0
HMF + 6 O2 → 6 CO2 + 3 water	1.0
Glucose-humins + 13.5 O2 → 12 CO2 + 4 water	1.0
Levulinic acid + 5.5 O2 → 5 CO2 + 4 water	1.0
Lignin (mixed) + 12.825 O2 → 10 CO2 + 6.95 water	1.0
ML + 7 O2 → 6 CO2 + 5 water	1.0
MMF + 7.5 O2 → 7 CO2 + 4 water	1.0
Rest (aq.) + 4.5 O2 → 6 CO2 + 4 water	1.0
Xylan (solid) + 5 O2 → 5 CO2 + 4 water	1.0
Xylose + 5 O2 → 5 CO2 + 5 water	1.0
Cellulose (solid) + 6 O2 → 6 CO2 + 5 water	1.0
Lignin (solid) + 12.825 O2 → 10 CO2 + 6.95 water	1.0
Rest (solid) + 4.5 O2 → 6 CO2 + 4 water	1.0
Xylose-humins + 13.5 O2 → 12 CO2 + 4 water	1.0
Methanol + 1.5 O2 → CO2 + 2 water	1.0

HRSG (countercurrent)

Cold stream outlet temperature = 430°C
Flue gas in = 870°C | flue gas out = 125°C
Water in = 20°C at 42 bar | steam out = 430°C at 42 bar

Medium pressure turbine

Outlet pressure = 12.5 bar
Case I = MWe output = 18MWe
Case II = MWe output = 19 MWe
Case III = MWe output = 22 MWe

Low pressure turbine

Outlet pressure = 0.025 bar
Case I = MWe output = 14 MWe
Case II = MWe output = 6 MWe
Case III = MWe output = 36 MWe

Reheat

Temperature in = 266°C
Temperature out = 350°C
Temp. out is controlled by design spec., so that liquid fraction of steam exiting low pressure steam turbine < 0.1

Condenser

Temperature = 21°C
Pressure = 0.025 bar | vapor fraction = 0

Pump

Outlet pressure = 42 bar

E.S.I., PART III: FLOWSHEET AND STREAM TABLES OF CASE I, II AND III

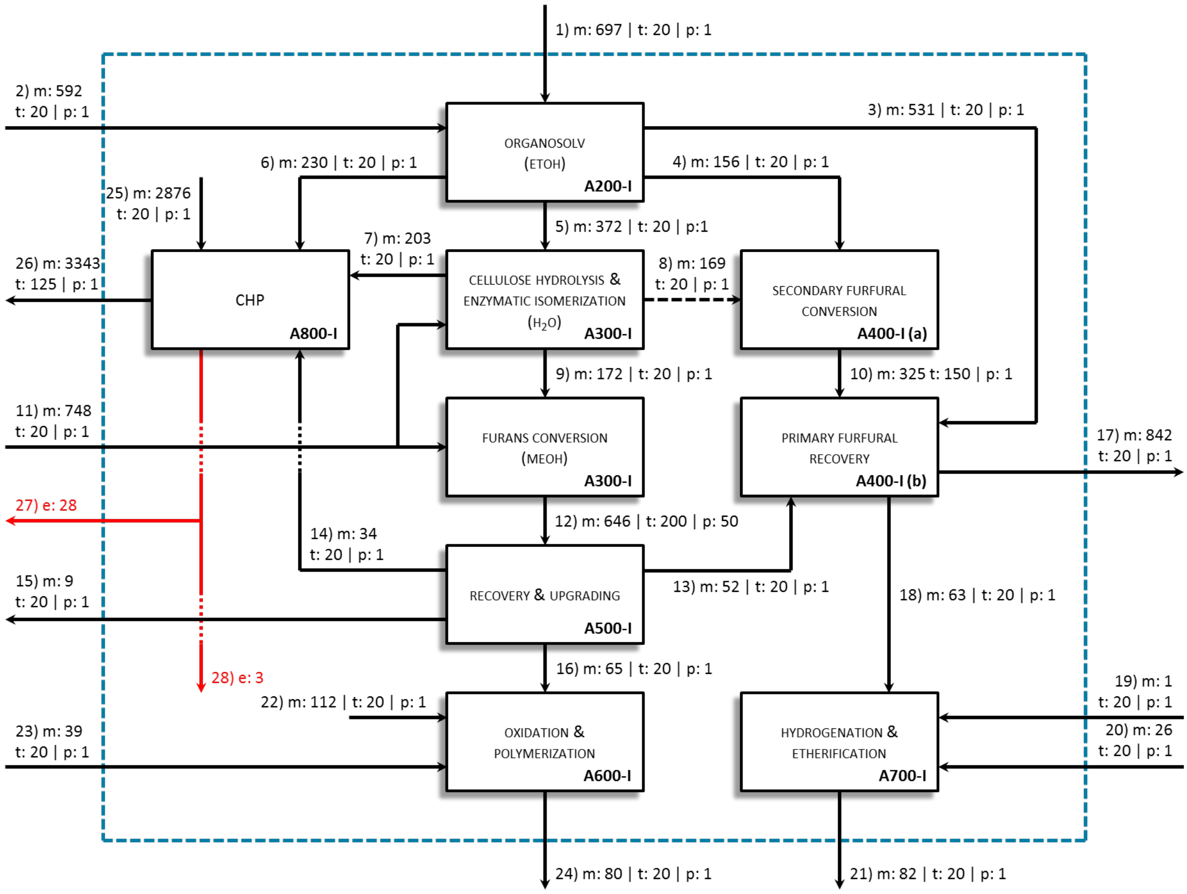

Figure 15: case I; flowsheet with mass flows, temperatures and pressures (internal recycling streams of ethanol and methanol not shown)

LIQUIDS (ktonnes/year)	1	2a, 2b	2c	2	3	4	5	6	7	8	9	10
Acetic acid	0	0	0	0	0	0	0	0	0	0	0	0
Cl-	0	0	0	0	0	1	0	1	0	0	0	1
CO_2	0	0	0	0	0	0	0	0	0	0	0	0
Dimethyl ether (DME)	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	0	3	0	3	3	0	0	0	0	0	0	0
Ethylene glycol	0	0	0	0	0	0	0	0	0	0	0	0
Formic acid	0	0	0	0	0	0	0	0	0	0	0	0
FDCA	0	0	0	0	0	0	0	0	0	0	0	0
FEE	0	0	0	0	0	0	0	0	0	0	0	0
Fructose	0	0	0	0	0	0	0	0	3	0	158	0
Furfural	0	0	0	0	41	2	0	2	0	0	0	19
Glucose	0	0	0	0	0	0	0	0	78	0	10	0
Hydrogen (H_2)	0	0	0	0	0	0	0	0	0	0	0	0
Sulfuric acid	0	0	4	4	0	1	0	2	0	0	0	1
HMF	0	0	0	0	0	0	0	0	0	0	0	0
Humins from glucose	0	0	0	0	0	0	0	0	0	0	0	0
Humins from xylose	0	0	0	0	0	0	0	0	0	0	0	0
K+	0	0	0	0	0	1	0	1	0	0	0	1
Levulinic acid	0	0	0	0	0	0	0	0	0	0	0	0
Lignin (dissolved)	0	0	0	0	0	4	12	4	12	0	0	4
Methanol	0	0	0	0	0	0	0	0	0	0	0	0
Methylal	0	0	0	0	0	0	0	0	0	0	0	0
Methyl formate (MF)	0	0	0	0	0	0	0	0	0	0	0	0
Methyl levulinate	0	0	0	0	0	0	0	0	0	0	0	0
MMF	0	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0	0
PEF	0	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (dissolved)	0	0	0	0	0	36	12	37	12	0	0	36
Water	73	585	0	585	487	89	0	92	2	138	4	237
Xylose	0	0	0	0	0	22	7	23	7	31	0	27
Subtotal LIQUIDS (ktonnes/year)	73	588	4	592	531	156	32	161	114	169	172	325

LIQUIDS (ktonnes/year)	11a	11b	11c	11d	11e	11f	11	12	13	14	15	16
Acetic acid	0	0	0	0	0	0	0	0	0	0	0	0
Cl-	0	0	0	0	0	0	0	0	0	0	0	0
CO2	0	0	0	0	0	0	0	8	0	0	0	0
Dimethyl ether (DME)	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	0	0	0	0	0	0	0	0	0	0	0	0
Ethylene glycol	0	0	0	0	0	0	0	0	0	0	0	0
Formic acid	0	0	0	0	0	0	0	3	2	0	0	0
FDCA	0	0	0	0	0	0	0	0	0	0	0	0
FEE	0	0	0	0	0	0	0	0	0	0	0	0
Fructose	0	0	0	0	0	0	0	1	0	1	0	0
Furfural	0	0	0	0	0	0	0	2	2	0	0	0
Glucose	0	0	0	0	0	0	0	0	0	0	0	0
Hydrogen (H2)	0	0	0	0	0	0	0	0	0	0	0	0
Sulfuric acid	0	0	0	0	1	0	1	1	0	1	0	0
HMF	0	0	0	0	0	0	0	11	0	11	0	0
Humins from glucose	0	0	0	0	0	0	0	20	0	20	0	0
Humins from xylose	0	0	0	0	0	0	0	0	0	0	0	0
K+	0	0	0	0	0	0	0	0	0	0	0	0
Levulinic acid	0	0	0	0	0	0	0	1	0	1	0	0
Lignin (dissolved)	0	0	0	0	0	0	0	0	0	0	0	0
Methanol	0	0	0	0	0	449	449	430	0	0	0	0
Methylal	0	0	0	0	0	0	0	2	0	0	0	0
Methyl formate (MF)	0	0	0	0	0	0	0	1	0	0	0	0
Methyl levulinate	0	0	0	0	0	0	0	9	0	0	9	0
MMF	0	0	0	0	0	0	0	65	0	1	0	65
Nitrogen	0	0	0	0	0	0	0	0	0	0	0	0
PEF	0	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (dissolved)	0	0	0	0	0	0	0	0	0	0	0	0
Water	436	418	354	226	0	24	298	91	48	0	0	0
Xylose	0	0	0	0	0	0	0	0	0	0	0	0
Subtotal LIQUIDS (ktonnes/year)	436	418	354	226	1	473	748	646	52	34	9	65

LIQUIDS (ktonnes/year)	17	18	19	20	21	22	23a	23b	23	24	25	26
Acetic acid	0	0	0	0	0	0	12	0	12	0	0	0
Cl-	1	0	0	0	0	0	0	0	0	0	0	1
CO_2	0	0	0	0	0	0	0	0	0	0	0	677
Dimethyl ether (DME)	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	0	0	0	26	1	0	0	0	0	0	0	0
Ethylene glycol	0	0	0	0	0	0	0	27	27	0	0	0
Formic acid	2	0	0	0	0	0	0	0	0	0	0	0
FDCA	0	0	0	0	0	0	0	0	0	0	0	0
FEE	0	0	0	0	70	0	0	0	0	0	0	0
Fructose	0	0	0	0	0	0	0	0	0	0	0	0
Furfural	0	63	0	0	2	0	0	0	0	0	0	0
Glucose	0	0	0	0	0	0	0	0	0	0	0	0
Hydrogen (H_2)	0	0	1	0	0	0	0	0	0	0	0	0
Sulfuric acid	2	0	0	0	0	0	0	0	0	0	0	3
HMF	0	0	0	0	0	0	0	0	0	0	0	0
Humins from glucose	0	0	0	0	0	0	0	0	0	0	0	0
Humins from xylose	0	0	0	0	0	0	0	0	0	0	0	0
K+	1	0	0	0	0	0	0	0	0	0	0	1
Levulinic acid	0	0	0	0	0	0	0	0	0	0	0	0
Lignin (dissolved)	4	0	0	0	0	0	0	0	0	0	0	0
Methanol	0	0	0	0	0	0	0	0	0	0	0	0
Methylal	0	0	0	0	0	0	0	0	0	0	0	0
Methyl formate (MF)	0	0	0	0	0	0	0	0	0	0	0	0
Methyl levulinate	0	0	0	0	0	0	0	0	0	0	0	0
MMF	0	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	88	0	0	0	0	2272	2272
PEF	0	0	0	0	0	0	0	0	0	80	0	0
Oxygen	0	0	0	0	0	23	0	0	0	0	604	60
Unknowns (dissolved)	36	0	0	0	0	0	0	0	0	0	0	0
Water	771	0	0	0	10	0	0	0	0	0	0	295
Xylose	27	0	0	0	0	0	0	0	0	0	0	0
Subtotal LIQUIDS (ktonnes/year)	842	63	1	26	83	112	0	0	39	80	2876	3308

SOLIDS (ktonnes/year)	1	2a, 2b	2c	2	3	4	5	6	7	8	9	10
Cellulose	236	0	0	0	0	0	236	0	12	0	0	0
KCl	3	0	0	0	0	0	0	0	0	0	0	0
Lignin (solid)	111	0	0	0	0	0	22	69	22	0	0	0
Unknowns (solids, but soluble)	85	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solid, insoluble)	19	0	0	0	0	0	19	0	19	0	0	0
SiO2	35	0	0	0	0	0	35	0	35	0	0	0
Xylan	136	0	0	0	0	0	27	0	0	0	0	0
Subtotal SOLIDS (ktonnes/year)	625	0	0	0	0	0	340	69	88	0	0	0
Total LIQ + SOL (ktonnes/year)	697	588	4	592	531	156	372	230	203	169	172	325
CONDITIONS												
Temperature (°C)	20	20	20	20	20	20	20	20	20	20	155	150
Pressure (bar)	1	1	1	1	1	1	1	1	1	1	1	5

SOLIDS (ktonnes/year)	11a	11b	11c	11d	11e	11f	11	12	13	14	15	16
Cellulose	0	0	0	0	0	0	0	0	0	0	0	0
KCl	0	0	0	0	0	0	0	0	0	0	0	0
Lignin (solid)	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solids, but soluble)	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solid, insoluble)	0	0	0	0	0	0	0	0	0	0	0	0
SiO2	0	0	0	0	0	0	0	0	0	0	0	0
Xylan	0	0	0	0	0	0	0	0	0	0	0	0
Subtotal SOLIDS (ktonnes/year)	0	0	0	0	0	0	0	0	0	0	0	0
Total LIQ + SOL (ktonnes/year)	436	418	354	226	1	473	748	646	52	34	9	65
CONDITIONS												
Temperature (°C)	20	20	20	20	20	20	20	200	20	20	20	20
Pressure (bar)	1	1	1	1	1	1	1	50	1	1	1	1

SOLIDS (ktonnes/year)	17	18	19	20	21	22	23a	23b	23	24	25	26
Cellulose	0	0	0	0	0	0	0	0	0	0	0	0
KCl	0	0	0	0	0	0	0	0	0	0	0	0
Lignin (solid)	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solids, but soluble)	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solid, insoluble)	0	0	0	0	0	0	0	0	0	0	0	0
SiO2	0	0	0	0	0	0	0	0	0	0	0	35
Xylan	0	0	0	0	0	0	0	0	0	0	0	0
Subtotal SOLIDS (ktonnes/year)	0	0	0	0	0	0	0	0	0	0	0	35
Total LIQ + SOL (ktonnes/year)	842	63	1	26	82	112	12	27	39	80	2876	3343
CONDITIONS												
Temperature (°C)	20	20	20	50	12	20	20	20	20	20	20	125
Pressure (bar)	1	1	1	1	1	1	1	1	1	1	1	1

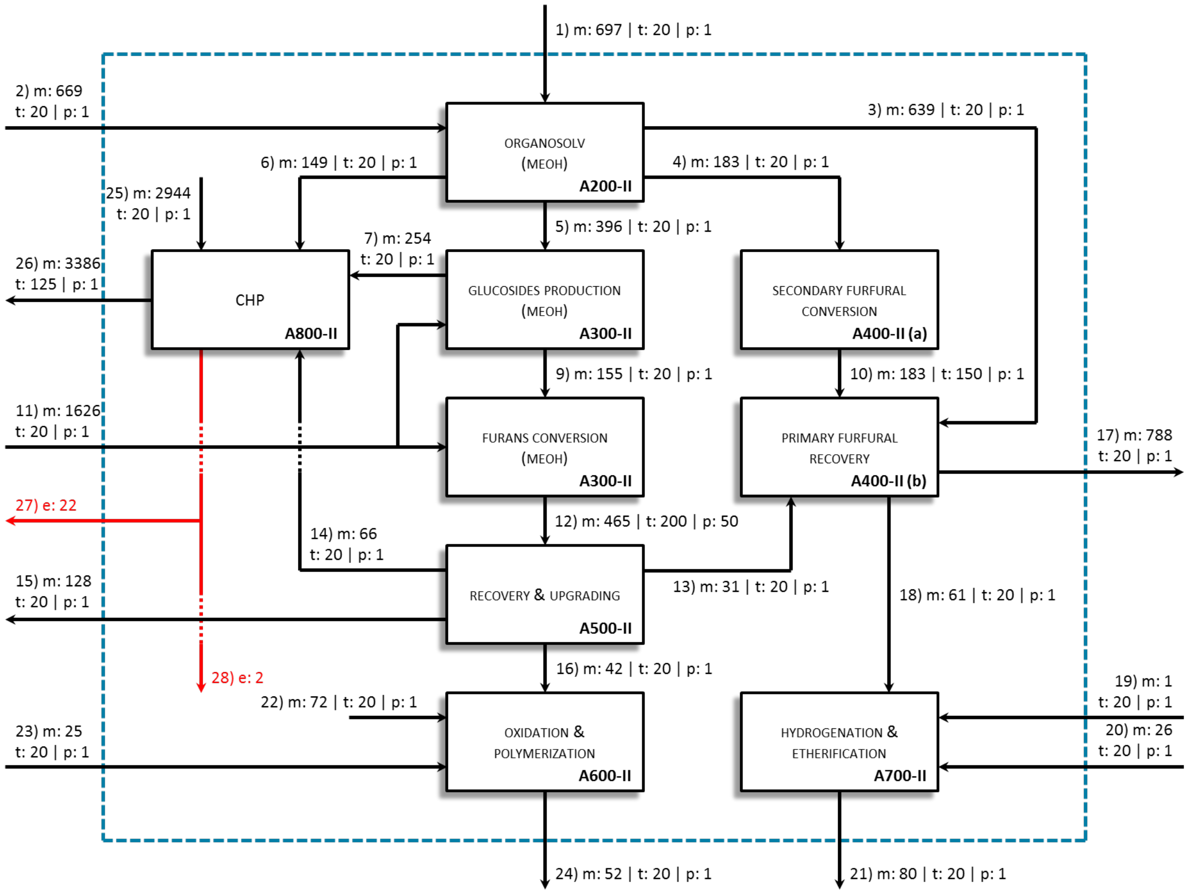

Figure 16: case II; flowsheet with mass flows, temperatures and pressures (internal recycling streams of methanol not shown)

LIQUIDS (ktonnes/year)	1	2a, 2b	2c	2	3	4	5	6	7	9	10	11a
Acetic acid	0	0	0	0	0	0	0	0	0	0	0	0
Cl-	0	0	0	0	0	1	0	0	0	0	1	0
CO_2	0	0	0	0	0	0	0	0	0	0	0	0
Dimethyl ether (DME)	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	0	0	0	0	0	0	0	0	0	0	0	0
Ethylene glycol	0	0	0	0	0	0	0	0	0	0	0	0
Formic acid	0	0	0	0	0	0	0	0	0	2	0	0
FDCA	0	0	0	0	0	0	0	0	0	0	0	0
FEE	0	0	0	0	0	0	0	0	0	0	0	0
Fructose	0	0	0	0	0	0	0	0	0	0	0	0
Furfural	0	0	0	0	42	3	0	1	0	7	11	0
Glucose	0	0	0	0	0	0	0	0	43	101	0	0
Hydrogen (H_2)	0	0	0	0	0	0	0	0	0	0	0	0
Sulfuric acid	0	0	4	4	0	2	0	1	0	0	2	0
HMF	0	0	0	0	0	0	0	0	1	6	0	0
Humins from glucose	0	0	0	0	0	0	0	0	0	0	0	0
Humins from xylose	0	0	0	0	0	0	0	0	0	0	0	0
K+	0	0	0	0	0	1	0	0	0	0	1	0
Levulinic acid	0	0	0	0	0	0	0	0	0	0	0	0
Lignin (dissolved)	0	0	0	0	0	7	11	4	9	2	7	0
Methanol	0	3	0	3	3	0	0	0	0	0	0	1250
Methylal	0	0	0	0	0	0	0	0	0	0	0	0
Methyl formate (MF)	0	0	0	0	0	0	0	0	0	0	0	0
Methyl levulinate	0	0	0	0	0	0	0	0	0	5	0	0
MMF	0	0	0	0	0	0	0	0	0	3	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0	0
PEF	0	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (dissolved)	0	0	0	0	0	45	14	26	4	10	45	0
Water	73	662	0	662	594	97	0	55	0	13	102	66
Xylose	0	0	0	0	0	28	8	16	3	6	14	0
Subtotal LIQUIDS (ktonnes/year)	73	665	4	669	639	183	34	104	61	155	183	1316

LIQUIDS (ktonnes/year)	11b	11c	11	12	13	14	15a	15b	15	16	17	18
Acetic acid	0	0	0	0	0	0	0	0	0	0	0	0
Cl-	0	0	0	0	0	0	0	0	0	0	1	0
CO2	0	0	0	5	0	0	0	0	0	0	0	0
Dimethyl ether (DME)	0	0	0	0	0	0	0	63	63	0	0	0
Ethanol	0	0	0	0	0	0	0	0	0	0	0	0
Ethylene glycol	0	0	0	0	0	0	0	0	0	0	0	0
Formic acid	0	0	0	4	1	0	0	0	0	0	1	0
FDCA	0	0	0	0	0	0	0	0	0	0	0	0
FEE	0	0	0	0	0	0	0	0	0	0	0	0
Fructose	0	0	0	0	0	0	0	0	0	0	0	0
Furfural	0	0	0	11	8	0	0	0	0	0	0	61
Glucose	0	0	0	0	0	0	0	0	0	0	0	0
Hydrogen (H2)	0	0	0	0	0	0	0	0	0	0	0	0
Sulfuric acid	0	1	1	1	0	1	0	0	0	0	2	0
HMF	0	0	0	13	0	13	0	0	0	0	0	0
Humins from glucose	0	0	0	12	0	12	0	0	0	0	0	0
Humins from xylose	0	0	0	1	0	1	0	0	0	0	0	0
K+	0	0	0	0	0	0	0	0	0	0	1	0
Levulinic acid	0	0	0	1	0	1	0	0	0	0	0	0
Lignin (dissolved)	0	0	0	2	0	2	0	0	0	0	7	0
Methanol	307	0	1557	295	0	0	0	0	0	0	0	0
Methylal	0	0	0	1	0	0	0	0	0	0	0	0
Methyl formate (MF)	0	0	0	1	0	0	0	0	0	0	0	0
Methyl levulinate	0	0	0	11	0	0	11	0	11	0	0	0
MMF	0	0	0	42	0	0	0	0	0	42	0	0
Nitrogen	0	0	0	0	0	0	0	0	0	0	0	0
PEF	0	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (dissolved)	0	0	0	10	0	10	0	0	0	0	45	0
Water	3	0	69	57	22	0	0	53	54	0	717	0
Xylose	0	0	0	0	0	0	0	0	0	0	14	0
Subtotal LIQUIDS (ktonnes/year)	310	1	1626	465	31	39	11	117	128	42	788	61

LIQUIDS (ktonnes/year)	19	20	21	22	23a	23b	23	24	25	26
Acetic acid	0	0	0	0	8	0	8	0	0	0
Cl-	0	0	0	0	0	0	0	0	0	1
CO_2	0	0	0	0	0	0	0	0	0	696
Dimethyl ether (DME)	0	0	0	0	0	0	0	0	0	0
Ethanol	0	26	0	0	0	0	0	0	0	0
Ethylene glycol	0	0	0	0	0	18	18	0	0	0
Formic acid	0	0	0	0	0	0	0	0	0	0
FDCA	0	0	0	0	0	0	0	0	0	0
FEE	0	0	80	0	0	0	0	0	0	0
Fructose	0	0	0	0	0	0	0	0	0	0
Furfural	0	0	0	0	0	0	0	0	0	0
Glucose	0	0	0	0	0	0	0	0	0	0
Hydrogen (H_2)	1	0	0	0	0	0	0	0	0	0
Sulfuric acid	0	0	0	0	0	0	0	0	0	2
HMF	0	0	0	0	0	0	0	0	0	0
Humins from glucose	0	0	0	0	0	0	0	0	0	0
Humins from xylose	0	0	0	0	0	0	0	0	0	0
K+	0	0	0	0	0	0	0	0	0	1
Levulinic acid	0	0	0	0	0	0	0	0	0	0
Lignin (dissolved)	0	0	0	0	0	0	0	0	0	0
Methanol	0	0	0	0	0	0	0	0	0	0
Methylal	0	0	0	0	0	0	0	0	0	0
Methyl formate (MF)	0	0	0	0	0	0	0	0	0	0
Methyl levulinate	0	0	0	0	0	0	0	0	0	0
MMF	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	57	0	0	0	0	2326	2326
PEF	0	0	0	0	0	0	0	52	0	0
Oxygen	0	0	0	15	0	0	0	0	618	62
Unknowns (dissolved)	0	0	0	0	0	0	0	0	0	0
Water	0	0	0	0	0	0	0	0	0	264
Xylose	0	0	0	0	0	0	0	0	0	0
Subtotal LIQUIDS (ktonnes/year)	1	26	80	72	8	18	25	52	2944	3352

SOLIDS (ktonnes/year)	1	2a, 2b	2c	2	3	4	5	6	7	9	10	11a
Cellulose	236	0	0	0	0	0	236	0	81	0	0	0
KCl	3	0	0	0	0	0	0	0	0	0	0	0
Lignin (solid)	111	0	0	0	0	0	45	45	45	0	0	0
Unknowns (solids, but soluble)	85	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solid, insoluble)	19	0	0	0	0	0	19	0	19	0	0	0
SiO2	35	0	0	0	0	0	35	0	35	0	0	0
Xylan	136	0	0	0	0	0	27	0	13	0	0	0
Subtotal SOLIDS (ktonnes/year)	625	0	0	0	0	0	362	45	193	0	0	0

Total LIQ + SOL (ktonnes/year)	697	665	4	669	639	183	396	149	254	155	183	1316

CONDITIONS												
Temperature (°C)	20	20	20	20	20	20	20	20	20	200	150	20
Pressure (bar)	1	1	1	1	1	1	1	1	1	50	5	1

SOLIDS (ktonnes/year)	11b	11c	11	12	13	14	15a	15b	15	16	17	18
Cellulose	0	0	0	0	0	0	0	0	0	0	0	0
KCl	0	0	0	0	0	0	0	0	0	0	0	0
Lignin (solid)	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solids, but soluble)	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solid, insoluble)	0	0	0	0	0	0	0	0	0	0	0	0
SiO2	0	0	0	0	0	0	0	0	0	0	0	0
Xylan	0	0	0	0	0	0	0	0	0	0	0	0
Subtotal SOLIDS (ktonnes/year)	0	0	0	0	0	0	0	0	0	0	0	0

Total LIQ + SOL (ktonnes/year)	310	1	1626	465	31	66	11	117	128	42	788	61

CONDITIONS												
Temperature (°C)	20	20	20	200	20	20	20	20	20	20	20	20
Pressure (bar)	1	1	1	50	1	1	1	1	1	1	1	1

SOLIDS (ktonnes/year)	19	20	21	22	23a	23b	23	24	25	26
Cellulose	0	0	0	0	0	0	0	0	0	0
KCl	0	0	0	0	0	0	0	0	0	0
Lignin (solid)	0	0	0	0	0	0	0	0	0	0
Unknowns (solids, but soluble)	0	0	0	0	0	0	0	0	0	0
Unknowns (solid, insoluble)	0	0	0	0	0	0	0	0	0	0
SiO2	0	0	0	0	0	0	0	0	0	35
Xylan	0	0	0	0	0	0	0	0	0	0
Subtotal SOLIDS (ktonnes/year)	0	0	0	0	0	0	0	0	0	35

Total LIQ + SOL (ktonnes/year)	1	26	80	72	8	18	25	52	2944	3386

CONDITIONS										
Temperature (°C)	20	50	14	20	20	20	20	20	20	125
Pressure (bar)	1	1	1	1	1	1	1	1	1	1

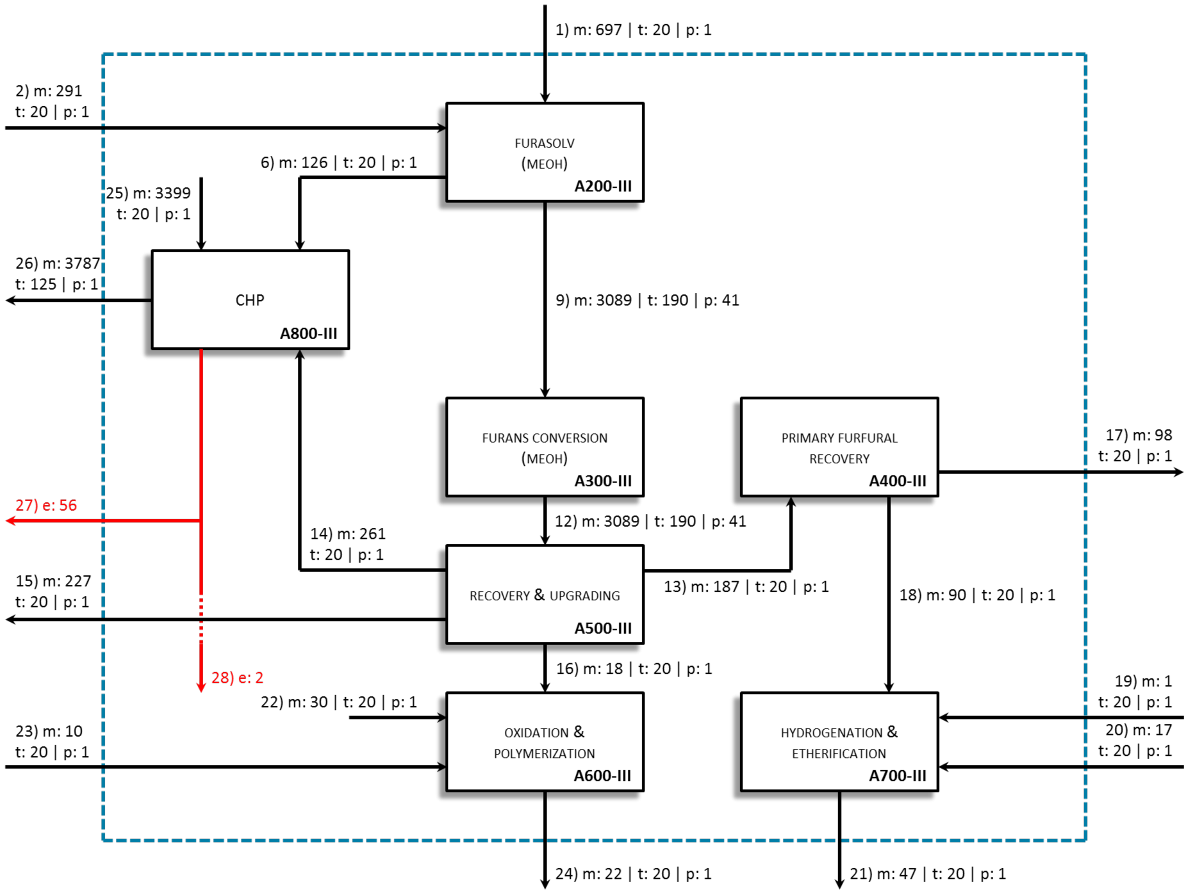

Figure 17: case III; flowsheet with mass flows, temperatures and pressures (internal recycling streams of methanol not shown)

LIQUIDS (ktonnes/year)	1	2a, 2b	2c	2	6	9	12	13	14	15a	15b	15	16
Acetic acid	0	0	0	0	0	0	0	0	0	0	0	0	0
Cl-	0	0	0	0	0	1	1	0	1	0	0	0	0
CO_2	0	0	0	0	0	26	35	0	0	0	0	0	0
Dimethyl ether (DME)	0	0	0	0	0	171	171	0	0	0	170	170	0
Ethanol	0	0	0	0	0	0	0	0	0	0	0	0	0
Ethylene glycol	0	0	0	0	0	0	0	0	0	0	0	0	0
Formic acid	0	0	0	0	0	0	0	0	0	0	0	0	0
FDCA	0	0	0	0	0	0	0	0	0	0	0	0	0
FEE	0	0	0	0	0	0	0	0	0	0	0	0	0
Fructose	0	0	0	0	0	0	0	0	0	0	0	0	0
Furfural	0	0	0	0	0	41	41	41	0	0	0	0	0
Glucose	0	0	0	0	9	106	20	0	20	0	0	0	0
Hydrogen (H_2)	0	0	0	0	0	0	0	0	0	0	0	0	0
Sulfuric acid	0	0	4	4	0	3	3	0	3	0	0	0	0
HMF	0	0	0	0	0	7	1	0	1	0	0	0	0
Humins from glucose	0	0	0	0	1	30	47	0	47	0	0	0	0
Humins from xylose	0	0	0	0	1	32	36	0	36	0	0	0	0
K+	0	0	0	0	0	2	2	0	2	0	0	0	0
Levulinic acid	0	0	0	0	0	0	0	0	0	0	0	0	0
Lignin (dissolved)	0	0	0	0	6	72	72	0	72	0	0	0	0
Methanol	0	269	0	269	0	2122	2106	0	0	0	0	0	0
Methylal	0	0	0	0	0	0	0	0	0	0	0	0	0
Methyl formate (MF)	0	0	0	0	0	26	38	0	0	0	0	0	0
Methyl levulinate	0	0	0	0	0	29	56	0	0	56	0	56	0
MMF	0	0	0	0	0	6	18	0	0	0	0	0	17
Nitrogen	0	0	0	0	0	0	0	0	0	0	0	0	0
PEF	0	0	0	0	0	0	0	0	0	0	0	0	0
Oxygen	0	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (dissolved)	0	0	0	0	6	78	78	0	78	0	0	0	0
Water	73	19	0	19	0	327	363	146	0	0	0	0	0
Xylose	0	0	0	0	1	10	0	0	0	0	0	0	0
Subtotal LIQUIDS (ktonnes/year)	73	288	4	291	25	3089	3089	187	261	56	170	227	18

LIQUIDS (ktonnes/year)	17	18	19	20	21	22	23a	23b	23	24	25	26
Acetic acid	0	0	0	0	0	0	3	0	3	0	0	0
Cl-	0	0	0	0	0	0	0	0	0	0	0	1
CO2	0	0	0	0	0	0	0	0	0	0	0	796
Dimethyl ether (DME)	0	0	0	0	0	0	0	0	0	0	0	0
Ethanol	0	0	0	26	11	0	0	0	0	0	0	0
Ethylene glycol	0	0	0	0	0	0	0	7	7	0	0	0
Formic acid	0	0	0	0	0	0	0	0	0	0	0	0
FDCA	0	0	0	0	0	0	0	0	0	0	0	0
FEE	0	0	0	0	47	0	0	0	0	0	0	0
Fructose	0	0	0	0	0	0	0	0	0	0	0	0
Furfural	5	35	0	0	0	0	0	0	0	0	0	0
Glucose	0	0	0	0	0	0	0	0	0	0	0	0
Hydrogen (H2)	0	0	1	0	0	0	0	0	0	0	0	0
Sulfuric acid	0	0	0	0	0	0	0	0	0	0	0	4
HMF	0	0	0	0	0	0	0	0	0	0	0	0
Humins from glucose	0	0	0	0	0	0	0	0	0	0	0	0
Humins from xylose	0	0	0	0	0	0	0	0	0	0	0	0
K+	0	0	0	0	0	0	0	0	0	0	0	2
Levulinic acid	0	0	0	0	0	0	0	0	0	0	0	0
Lignin (dissolved)	0	0	0	0	0	0	0	0	0	0	0	0
Methanol	0	0	0	0	0	0	0	0	0	0	0	0
Methylal	0	0	0	0	0	0	0	0	0	0	0	0
Methyl formate (MF)	0	0	0	0	0	0	0	0	0	0	0	0
Methyl levulinate	0	0	0	0	0	0	0	0	0	0	0	0
MMF	0	0	0	0	0	0	0	0	0	0	0	0
Nitrogen	0	0	0	0	0	24	0	0	0	0	2685	2685
PEF	0	0	0	0	0	0	0	0	0	22	0	0
Oxygen	0	0	0	0	0	6	0	0	0	0	714	71
Unknowns (dissolved)	0	0	0	0	0	0	0	0	0	0	0	0
Water	92	54	0	0	24	0	0	0	0	0	0	192
Xylose	0	0	0	0	0	0	0	0	0	0	0	0
Subtotal LIQUIDS (ktonnes/year)	98	90	1	26	82	30	3	7	10	22	3399	3752

SOLIDS (ktonnes/year)	1	2a, 2b	2c	2	6	9	12	13	14	15a	15b	15	16
Cellulose	236	0	0	0	14	0	0	0	0	0	0	0	0
KCl	3	0	0	0	0	0	0	0	0	0	0	0	0
Lignin (solid)	111	0	0	0	33	0	0	0	0	0	0	0	0
Unknowns (solids, but soluble)	85	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solid, insoluble)	19	0	0	0	19	0	0	0	0	0	0	0	0
SiO2	35	0	0	0	35	0	0	0	0	0	0	0	0
Xylan	136	0	0	0	0	0	0	0	0	0	0	0	0
Subtotal SOLIDS (ktonnes/year)	625	0	0	0	102	0	0	0	0	0	0	0	0
Total LIQ + SOL (ktonnes/year)	697	288	4	291	126	3089	3089	187	261	56	170	227	18
CONDITIONS													
Temperature (°C)	20	20	20	20	20	190	200	20	20	20	20	20	20
Pressure (bar)	1	1	1	1	1	41	41	1	1	1	1	1	1

SOLIDS (ktonnes/year)	17	18	19	20	21	22	23a	23b	23	24	25	26
Cellulose	0	0	0	0	0	0	0	0	0	0	0	0
KCl	0	0	0	0	0	0	0	0	0	0	0	0
Lignin (solid)	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solids, but soluble)	0	0	0	0	0	0	0	0	0	0	0	0
Unknowns (solid, insoluble)	0	0	0	0	0	0	0	0	0	0	0	0
SiO2	0	0	0	0	0	0	0	0	0	0	0	35
Xylan	0	0	0	0	0	0	0	0	0	0	0	0
Subtotal SOLIDS (ktonnes/year)	0	0	0	0	0	0	0	0	0	0	0	35
Total LIQ + SOL (ktonnes/year)	98	90	1	17	47	30	3	7	10	22	3399	3787
CONDITIONS												
Temperature (°C)	20	20	20	20	20	20	20	20	20	20	20	125
Pressure (bar)	1	1	1	1	1	1	1	1	1	1	1	1