DOPO production from CDOP [35948-25-5]

CONTENTS OF FACTORY GATE TO FACTORY GATE

LIFE CYCLE INVENTORY SUMMARY

Authors	Z. Hu and J. Harris
Peer reviews, name (date)	Reviewed by MRO on 6-6-2011: route, stoichiometry, and calculations reviewed and found to be representative.
Gtg report last modified on	7-29-2022
Additional notes	

Checked for database consistency on	6-6-2011
First gtg version finalized on	4-25-2011
Modification history, Author (date)	JLH (7-29-2022) and ZH (6-6-2011)

Products	DOPO, Hydrogen chloride
Standard inputs	CDOP, Water

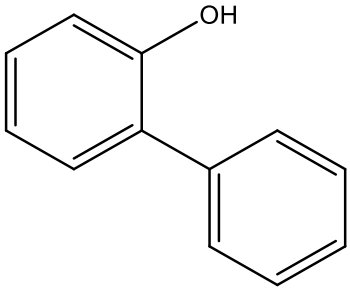
Methodology: Environmental Clarity gtg lci reports are based on industrial practice information, standard methods of engineering process design, and technical reviews. These reports are intended to be representative of industrial production based on the stated route.

Terms of use: Environmental Clarity does not assume any liability due to use of these lci data. Integration of these data with lci data based on other methodologies is the responsibility of the user. Each report may be updated to improve model accuracy or representativeness.

Users of this report should cite: E. Griffing and M. Overcash, Chemical Life Cycle Database, www.environmentalclarity.com, 1999 - present.

Chemistry

Primary reaction:		
	$C_{12}H_{10}O + PCl_3 \rightarrow C_{12}H_8ClOP + 2HCl$	(1)
	$2H_2O + C_{12}H_8ClOP \rightarrow C_{12}H_{11}O_3P + HCl$	(2)
	$C_{12}H_{11}O_3P \rightarrow C_{12}H_9O_2P + H_2O$	(3)
Net reaction:	$C_{12}H_{10}O + PCl_3 + H_2O \rightarrow C_{12}H_9O_2P + 3HCl$	(4)

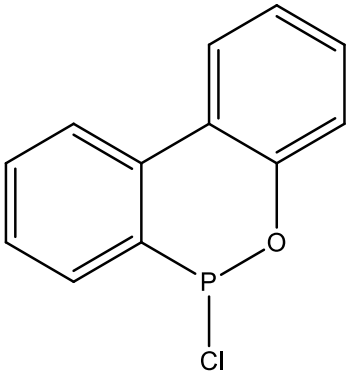


o-Phenylphenol

$C_{12}H_{10}O$

90-43-7

OPP

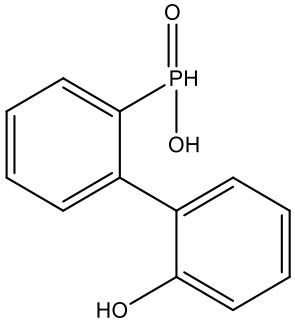


6-chloro-6H-dibenzo[c,e][1,2]oxaphosphinine

$C_{12}H_8$ ClOP

22749-43-5

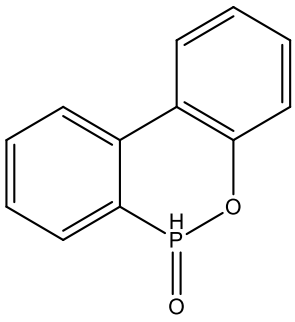
CDOP



(2'-hydroxy-[1,1'-biphenyl]-2-yl)phosphinic acid

Chemical Formula: $C_{12}H_{11}O_3P$

HPPA



9,10-Dihydro-9-oxa-10-phosphaphenanthrene 10-oxide

$C_{12}H_9O_2P$

35948-25-5

DOPO

Literature

The following are descriptions from various sources that are used in a consolidated fashion to convert CDOP to DOPO

CN 1709897A

Four steps to get DOPO

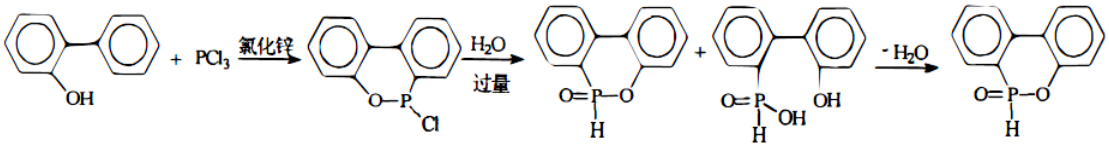
1. OPP + PCl3 under catalyst lewis acid, usually ZnCl2, to get CDOP at temperature 169-180 degree for 8-10 hours and purify with filter. Molar ratio for OPP:PCl3=1:1.25-1:1.35
2. Hydrolysis of CDOP to get HPPA, remove HCl. The molar ratio of water:opp = 1.2-2.5 for 1-4 hours. The CDOP fully convert to HPPA.
3. Wash the HPPA with alcohols to remove impurity. The mass ratio for alcohol: opp = 0.3-1.2 to remove excess Zn+ in the solution to make sure Zn+ less than 10ppm and crystallize the products.
4. Subatomspheric distillation to remove water in HPPA to synthesize DOPO. Temperature 110-125 degree.

For the first step, the CDOP lci gtg should be consulted.

For the second step: CDOP is direct hydrolyzed in an aromatic hydrocarbon solution, at a temperature of 70-105 degree. The product is HPPA and small amount of DOPO.

For the third step: the mixture is washed with alcohol and crystallize the HPPA.

For the forth step: distillation at 110-135 degree and > 90kPa to remove excess water in the HPPA and then cooling down to 20-22 degree. Conversion ratio: 92%, melting point 117-119 C, Zn+: 8ppm. Purity: >98.6%



Several examples are listed in the patent.

CN 101108864A

1. PCl3+OPP under ZnCl2 at temperature to get CDOP
2. Distillate the excess PCl3, then get rid of impurity by filtration. Then vaccum distillation to get CDOP distillate.
3. Hydrolysis of CDOP to get DOPO.

Detailed Information for each step

1. OPP:PCl3 = 1:1.5 – 1:2 molar ratio (recommended 1:1.2 mol). ZnCl2:OPP mass = 0.2-1%. Reaction is carried out at 180 C. The ratio for HCl and PCl3 in vented gas is 1:0.13 mole
2. Mixed with equal volume dimethylbenzene and distillate the PCl3 at 0.05 – 0.06 mPa, filter to remove impurity, and then remove water from CDOP under vacuum distillation under 0.17 kPa, 160-165 degree.
3. CDOP mixed with equal volume dimethylbenzene and water, the molar ratio for CDOP:H2O is 1:2-2.5. Then hydrolyze CDOP at 80 degree to get DOPO.

Five examples are given in this patent.

CN 1911941A

Polymer, 1998, 39(23):5819-5826

1. Synthesis of CDOP

2. OPP and PCl3 are mixed and then heated to 50 degree. The reaction mixture was heated at reflux (145 degree) until HCl evolution has subsided. The mixture was further heated at reflux temperature for another 5 h with addition of zinc chloride. The reaction was assumed to be complete when no more HCl evolution was detected at 210 degree.
3. Excess PCl3 was removed under vacuum and the residual solid was recrystallized from tetrahydrofuran to give CDOP. (yield 95%, mp 84-85 degree)
4. CDOP was preheated to 100 degree and deionized water is added with stirring. The mixture was stirred at 100 C to precipitate white solids which were filtered. The filtered solids were stirred with deionized water and aqueous NaoH solution until all solids were dissolved. The solution was heated at 50 degree, and then H2SO4 was added to neutralize NaOH. The precipitated solid HPPA was collected by filtration and thoroughly washed with H2O and dried.
5. HPPA is heated to molten state (106 degree) and the temperature is slowly increased from 106 to 160 degree until the dehydration was complete until the dehydration was complete. White solids of DOPO (yield 93%) with mp 119-120 degree are produced after recrystallization.

Synthesis and Application of DOPO

There are two routines for production of DOPO. One is through synthesis, another is through hydrolysis. Satio etc suggested a synthesis routine. Excess PCl3 is added to OPP, and then catalyst is added after the temperature reached 140 C. Hydrolysis to get DOPO after temperature reaches 170-220 C. Vacuum distillation is used to purify the DOPO. Kleiner improved this routine by adding excess PCl3 into OPP and catalysis gradually. Heated the solution to 180-220 C, and then hydrolyze to get DOPO. The routine takes 4-6 hours and excess PCl3.

以 2-羟基联苯(OPP)和三氯化磷为原料,采用两步法合成了新型阻燃剂中间体 2'-羟基联苯基-2-次膦酸(HBP).通过正交实验确定的适宜工艺条件 为:m(催化剂):m(OPP)=0.006:1,n(PCl3):n(OPP)=1.4:1;PCl3 先在 80℃滴加 70%,剩余部分在 180℃滴加, 然后升温到 220℃并维持反应 2 h.在上述条件下,OPP 的转化率达 99%以上,HBP 收率达 93%以上,产物经熔点测定和红外表征确认.

US6107506 – PROCESS FOR PRODUCING 2-(2-HYDROXYPHENYL) PHENYLPHOSPHING ACID AND DERIVATIVES

1. CDOP production: mole ratio of OPP and the phosphorus trichloride is about 1:1~2, preferably about 1:1.1~1.5. The amount of the catalyst used is about 0.05~3 parts by weight (hereinafter referred to “part”), preferably about 0.1~1 parts to 100 parts of OPP with reaction temperature about 30 ~ 250 C.
2. After completion of the condensation reaction, the reaction mixture is cooled to 80~90 C, and added to an organic solvent which is insoluble in water and is inert in the reaction system to dissolve the reaction mixture. The amount of the solvent is about 30~100 parts, preferably about 40~70 parts to 100 parts of OPP.
3. The mixed solution is cooled to about 35 C or less and then gradually poured into the liquid mixture of water and solvent with stirring. The temperature is elevated 15 ~ 30 C, the amount of water is a 5-20 molar excess of water based on OPP, and the solvent is 100 ~ 500 parts to 100 parts of OPP.
4. After the completion of the hydrolysis reaction, the reaction liquid mixture is cooled to 60~90 C, and allowed to stand, followed by separation of a water layer and oil layer for three times. The amount of warm water is preferably 0.3-0.6 times the reaction liquid mixture.
5. After water washing, residual moisture of the oil layer is removed by azeotropic distillation, and the decoloration treatment is conducted at 70~80 C.
6. After filtration, preferably 40-70 parts of water is added to cool about 25 C or less, followed by filtration and washing of the precipitates to obtain white crystalline, wet filtration mass.
7. The wet filtration mass, a cyclic dehydration reaction is carried out under reduced pressure 110 mmhG at 110-180 C.

Example 1: PCl3:OPP (molar ratio) = 1.5:1.2 =1.25:1

Chemical Properties

	Mp (C)	Density	bp
CDOP	87		
DOPO	118 (206 - flash point)	1.39	200 (1mmHg), 399.66 (760mmHg)

	CN1709897A	CN101108864A	This design
CDOP Wash	Toluene 0.4-1.2 of OPP (m)	Toluene 1 of OPP (v)	Toluene of 0.8 OPP Mass
H2O:OPP (n)	2-4	2-2.5	2.2
Temperature	70-105 C	80	80
HPPA wash and filter	Alcohol 0.3-1.2 (m)/OPP to remove Zn2+	Toluene	Toluene
Vacuum Distillation	>90 kPa	vacuum	0.13 atm
	110-135 C		140 C

LCI design

This design is principally based on patent US6,107,506. CDOP is mixed with toluene, which is insoluble in water and is inert in the reaction system. The amount of toluene is 0.5 times of the mass of CDOP. This mixed solution is cooled to 35 C, and then gradually poured into the liquid mixture of water and solvent with stirring. After the completion of hydrolysis reaction, the reaction liquid mixture is cooled to 80 C. and allowed to sand, followed by separation of water layer and then, water of 70 C is added to an oil layer and stirred and allowed to stand, followed by separation of liquid (90% of catalyst is removed in the aqueous stream. This washing operation for the organic phase is repeated for 2 times with each wash removing 90% of the input catalyst to reach a level of 0.1% catalyst. The amount of warm water is 0.5 times the reaction liquid mixture. Then clay is added to oil layer to remove impurity, the step is called decoloring. Then, this mixture is further cooled to 25 C or less, followed by filtration to get wet HPPA product (25 wt% toluene). Then for this wet HPPA, a cyclic dehydration reaction is carried out under reduced pressure at 140 degree and 100 mmHg to remove water and toluene. The overhead gas stream of toluene and water is recycled to R1. After the cyclising dehydration reaction, the contents are poured out to a flaker and cooled to 100 C to achieve the desired product form (25 hp per 1000 kg flake/hr, http://sunderengineeringworks.com). The product then cools to 25C under ambient conditions, to get the final product, DOPO.

References

Zhengmao Zhou, Lijun Qian etc., Synthesis of compound 9,10-dihydro-9-oxy-10-phospha phenanthrene and purification process thereof, CN 1709897 (A), 2005
Baoqing Wu, Xuejun Guo, etc., 9,10-dihydro-9-oxa-10-phosphine hetero-phenanthrene-10-oxide compound and its derivant and method of preparing the same, CN101108864 (A), 2008

Xiaoyan Gu, Preparation method of 2,10-dihydro-9-oxa-10-phospho hetero phenanthrene, CN 1911941 (A), 2007
Chun-shan, Wang and Jeng-Yueh Shieh, Synthesis and properties of epoxy resins containing 2-(6-oxid-6H-dibenz<c,e><1,2>oxaphosphorin-6-yl)1,4-benzenediol, Polymer, vol 39, No. 23, pp 5819-5826
Jianzhong Jiang and Chun Cai, Synthesis and Application of a Novel Flame Retardant Intermediate DOPO, Jiangsu Chemical Industry, 2004, 32 (1)
Toranosuke Saito, etc., Process for producing 2-(2-hydroxyphenyl)phenylphosphinic acid and detivates, US 6107506, 2000

Critical parameters

Conversion / Yield information from both reactors			
		Conversion of or Yield from CDOP	Conversion of or Yield from HPPA
Total conversion in reactor 1: (% of reactant entering the process that reacts)	From mass balance	100%	
Total per pass conversion in reactor 1: (% of reactant entering the reactor that reacts)	From mass balance	100%	
Total yield of reactor 1: (% yield ProductChem produced in the reactor based on reactant input to process)	From mass balance	99.50%	
Total conversion in reactor 2: (% of reactant entering the process that reacts)	From mass balance		100%
Total per pass conversion in reactor 2: (% of reactant entering the reactor that reacts)	From mass balance		100%
Total yield of reactor 2: (% yield produced in the reactor based on reactant input to process)	From mass balance		100%
Total yield of Process: (% yield produced by the overall process based on reactant input to process)	From mass balance	89.93%	
Notes:			

Product purity		
	ProductChem	Comments
Used here	99.1%	
LiteratureSource		

Summary of LCI Information

Standard inputs					
UID	Name	Flow	Purity	Units	Comments
22749-43-5	CDOP	1208	-	[kg/hr]	
7732-18-5	Water	102	-	[kg/hr]	
	Total	1310		[kg/hr]	
Non-reacting inputs					
UID	Name	Flow	Purity	Units	Comments
7732-18-5	Water	454	-	[kg/hr]	
108-88-3	Toluene	0.785	-	[kg/hr]	
7646-85-7	Zinc chloride	10.5	-	[kg/hr]	
	Total	465		[kg/hr]	
Ancillary inputs					
UID	Name	Flow	Purity	Units	Comments
	Total	0		[kg/hr]	
Products					
UID	Name	Flow	Purity	Units	Comments
35948-25-5	DOPO	1000	-	[kg/hr]	
7647-01-0	Hydrogen chloride	188	0.375	[kg/hr]	188 kg of HCl as 37.5% Solution
	Total	1188		[kg/hr]	
Benign outflows					
UID	Name	Flow	Purity	Units	Comments
7732-18-5	Water	454	-	[kg/hr]	313 kg included in HCl product
	Total	454		[kg/hr]	

Process emissions							
UID	Name	Gas	Liquid	Solid	Solvent	Units	Comments
UIDHPPA	HPPA	0	122	0	0	[kg/hr]	
35948-25-5	DOPO	0	0.202	0	0	[kg/hr]	
7647-01-0	Hydrogen chloride	0.940	0	0	0	[kg/hr]	
108-88-3	Toluene	7.14	0.371	0	0	[kg/hr]	
7646-85-7	Zinc chloride	0	10.5	0	0	[kg/hr]	
	Total	8.08	133	0	0		

Mass balance	
Total inputs	1775
Total outflows	1783
Net input	-7.68

Energy use			
Energy type	Amount	Units	Comments
electricity	92.1	[MJ/hr]	Net electricity use at plant
heating steam	1135	[MJ/hr]	heating by steam (0.85 efficiency included)
Net input requirement	1227	[MJ/hr]	Net of energies input to system
cooling water	-1182	[MJ/hr]	net cooling by cooling water
potential recovery	-295	[MJ/hr]	potential energy recovery (negative)
Net energy	931	[MJ/hr]	Net input requirement - potential recovery

Process Diagram Interpretation Sheet

1) As much as possible, standard symbols are used for all unit processes.

2) Only overall input and output chemicals are labeled on these diagrams. All intermediate information is given on the attached Process Mass Balance sheet

3) The physical state of most streams is shown (gas, g; liquid, l; solid, s)

4) The process numbering is as follows,

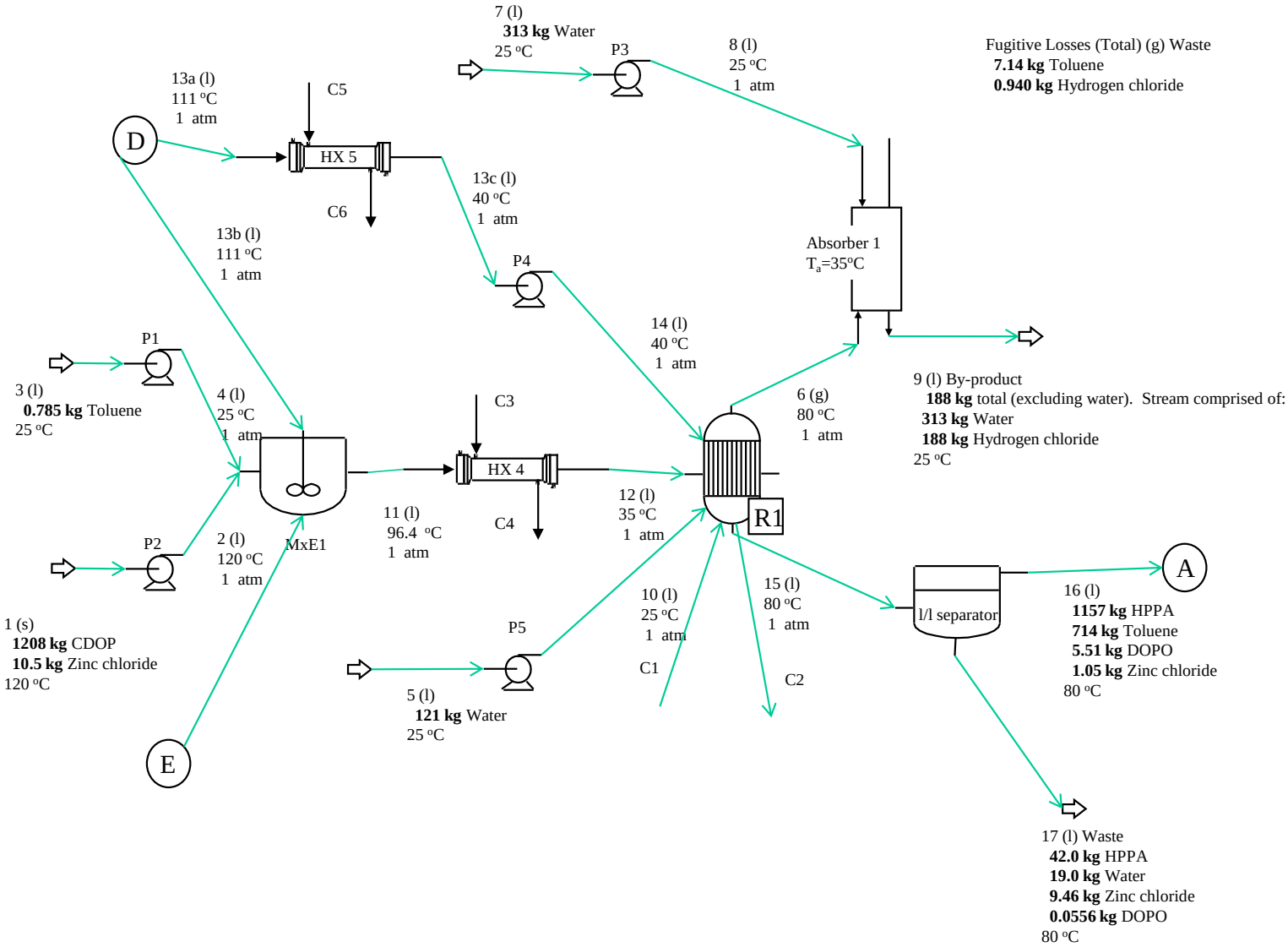
- generally numbers progress from the start to the end of the process
- numbers are used for process streams
- C i , i = 1,..n are used for all cooling non-contact streams
- S j, j = 1,...n are used for all steam heating non-contact streams

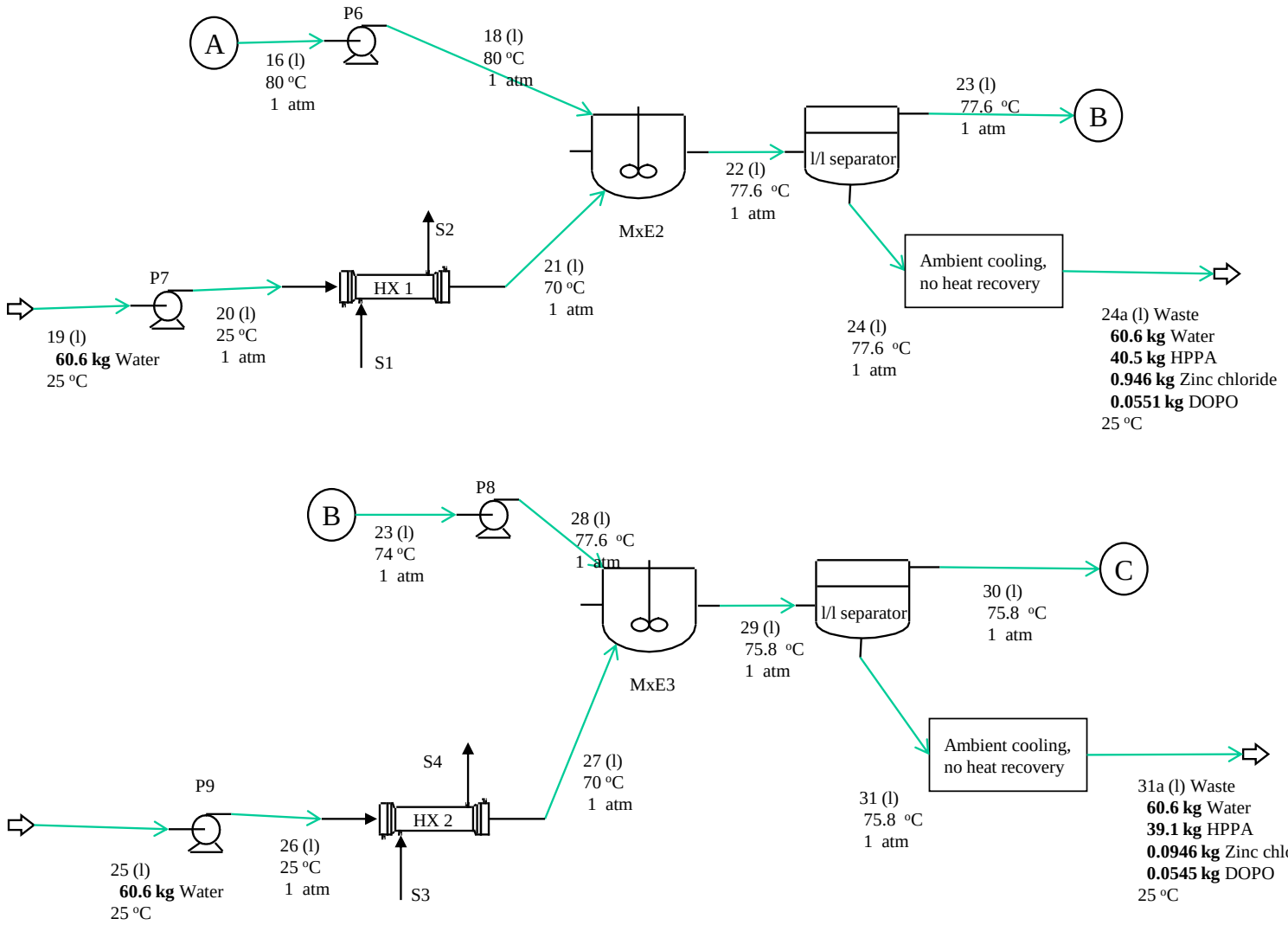
5) Recycle streams are shown with dotted lines

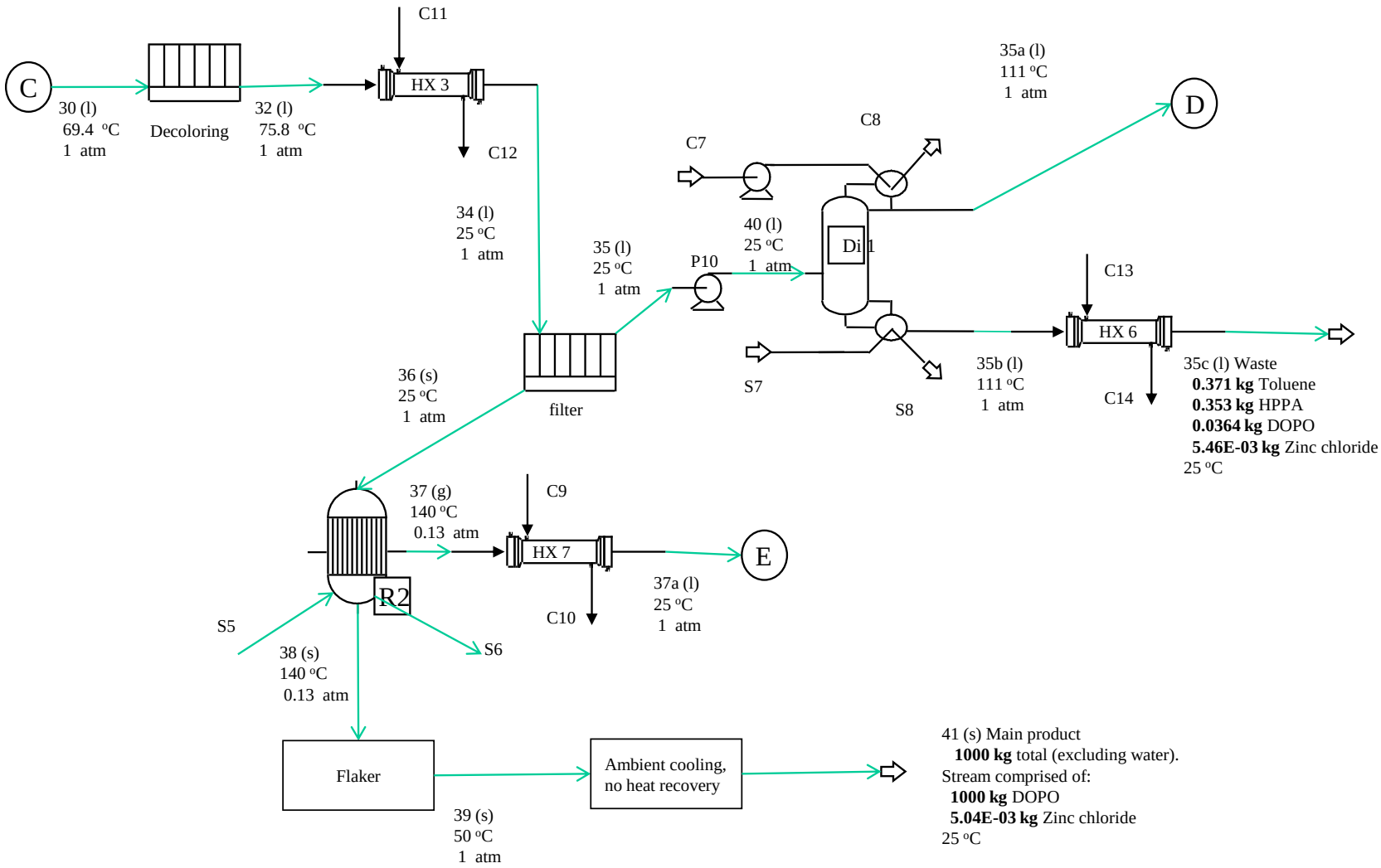
For most streams, the temperature and pressure are shown, if the pressures are greater than 1 atm

Process Diagram or Boundary of LCI

Steam enters the process as a gas at 207 ºC and leaves as a liquid at 207 ºC. Cooling water enters at 20 ºC and leaves at 50 ºC.
Unless




A
P6
16 (l)
80 °C
1 atm
18 (l)
80 °C
1 atm
MxE2
22 (l)
77.6 °C
1 atm
l/l separator
23 (l)
77.6 °C
1 atm
B
S2
HX 1
S1
P7
19 (l)
60.6 kg Water
25 °C
20 (l)
25 °C
1 atm
21 (l)
70 °C
1 atm
Ambient cooling,
no heat recovery
24 (l)
77.6 °C
1 atm
24a (l) Waste
60.6 kg Water
40.5 kg HPPA
0.946 kg Zinc chloride
0.0551 kg DOPO
25 °C
B
P8
23 (l)
74 °C
1 atm
28 (l)
77.6 °C
1 atm
MxE3
29 (l)
75.8 °C
1 atm
l/l separator
30 (l)
75.8 °C
1 atm
C
S4
HX 2
S3
P9
25 (l)
60.6 kg Water
25 °C
26 (l)
25 °C
1 atm
27 (l)
70 °C
1 atm
Ambient cooling,
no heat recovery
31 (l)
75.8 °C
1 atm
31a (l) Waste
60.6 kg Water
39.1 kg HPPA
0.0946 kg Zinc chloride
0.0545 kg DOPO
25 °C


C
30 (l)
69.4 °C
1 atm
Decoloring
32 (l)
75.8 °C
1 atm
C11
HX 3
C12
34 (l)
25 °C
1 atm
35 (l)
25 °C
1 atm
P10
C7
40 (l)
25 °C
1 atm
Di 1
C8
35a (l)
111 °C
1 atm
D
C13
HX 6
35b (l)
111 °C
1 atm
C14
35c (l) Waste
0.371 kg Toluene
0.353 kg HPPA
0.0364 kg DOPO
5.46E-03 kg Zinc chloride
25 °C
S7
S8
filter
36 (s)
25 °C
1 atm
37 (g)
140 °C
0.13 atm
C9
HX 7
E
37a (l)
25 °C
1 atm
C10
R2
S5
S6
38 (s)
140 °C
0.13 atm
Flaker
Ambient cooling,
no heat recovery
39 (s)
50 °C
1 atm
41 (s) Main product
1000 kg total (excluding water).
Stream comprised of:
1000 kg DOPO
5.04E-03 kg Zinc chloride
25 °C

Mass Balance of Chemicals in Each Process Stream

All flow rates are given in kg / hr.

Physical state of chemical losses: Gas, Liquid, Solid.

	Comments	Streams	Temp [C]	P	Phase	Total Flow	CDOP	HPPA	DOPO	Hydrogen chloride	Water	Toluene	Zinc chloride
Input		1	120	1.00	s	1219	1208						10.5
		2	120	1.00	l	1219	1208						10.5
Input		3	25.0	1.00	l	0.785						0.785	
		Stream 35a:Recycle input				265	0	0.0133	5.31E-04	0	0	265	0
		Stream 35a:Recycle calculated				265	0	0.0133	5.31E-04	0	0	265	0
		Stream 35a:Recycle residue				-0.0775	0	-3.88E-06	-1.55E-07	0	0	-0.0775	0
		Stream 37a:Recycle input				425	0	0	0	0	82.9	342	0
		Stream 37a:Recycle calculated				426	0	0	0	0	82.9	343	0
		Stream 37a:Recycle residue				-0.336	0	0	0	0	2.42E-05	-0.336	0
		13b	111	1.00	l	265	0	0.0133	5.31E-04	0	0	265	0
		13c	40.0	1.00	l	265	0	0.0133	5.31E-04	0	0	265	0
		4	25.0	1.00	l	0.793		7.99E-03	3.20E-04	0	0	0.785	
		11	96.4	1.00	l	1910	1208	0.0213	8.51E-04	0	82.9	608	10.5
		12	35.0	1.00	l	1910	1208	0.0213	8.51E-04	0	82.9	608	10.5
Input		5	25.0	1.00	l	121					121		
	5.15	10	25.0	1.00	l	121					121		

	Comments	Streams	Temp [C]	P	Phase	Total Flow	CDOP	HPPA	DOPO	Hydrogen chloride	Water	Toluene	Zinc chloride
		13a	111	1.00	l	106		5.28E-03	2.11E-04			106	
		14	40.0	1.00	l	106						106	
R1	1202	kg		CDOP	:	is converted in rxn (99.5 % of reactor input)							
	6.04	kg		CDOP	:	is converted in rxn (0.500 % of reactor input)							
		Input to reactor			:	2137	1208	0.0266	1.06E-03	0	204	714	10.5
		R1 Reaction Coefficient 1			:		-1.00	1.00		1.00	-2.00		
		R1 Conversion 1 [kg/hr]			:	0	-1202	1199		187	-185		
		R1 Conversion 1 [kgmol/hr]			:	5.13	-5.13	5.13		5.13	-10.3		
		R1 Reaction Coefficient 2			:		-1.00		1.00	1.00	-1.00		
		R1 Conversion 2 [kg/hr]			:	0	-6.04		5.56	0.940	-0.464		
		R1 Conversion 2 [kgmol/hr]			:	0.0258	-0.0258		0.0258	0.0258	-0.0258		
		Flow out of reactor			:	2137	-5.15E-14	1199	5.56	188	19.0	714	10.5
		Primary product			:	HPPA							
		Total conversion			:		100.0	NA	NA	NA	33.3	-0	-0
		Per pass conversion			:		100	NA	NA	NA	90.7	-0	-0
		Total yield from reactor			:		99.5	NA		NA	99.7		
		6	80.0	1.00	g	188				188			
Input		7	25.0	1.00	l	313					313		
		8	25.0	1.00	l	313					313		
By-product		9	25.0	1.00	l	-501				-188	-313		
		15	80.0	1.00	l	1948	-5.15E-14	1199	5.56		19.0	714	10.5
l/l sep <1>		percentage in oil phase			:			96.5	99.0		0	100	10.0
		percentage in aqueous phase			:			3.50	1.00		100	0	90.0
Display in PFD		16	80.0	1.00	l	1878	0	1157	5.51	0	0	714	1.05
Waste		17	80.0	1.00	l	-70.5		-42.0	-0.0556		-19.0	0	-9.46
		18	80.0	1.00	l	1878	0	1157	5.51	0	0	714	1.05
Input	657	19	25.0	1.00	l	60.6					60.6		
		20	25.0	1.00	l	60.6	0	0	0	0	60.6	0	0

	Comments	Streams	Temp [C]	P	Phase	Total Flow	CDOP	HPPA	DOPO	Hydrogen chloride	Water	Toluene	Zinc chloride
		21	70.0	1.00	l	60.6	0	0	0	0	60.6	0	0
		22	77.6	1.00	l	1939	0	1157	5.51	0	60.6	714	1.05
l/l sep <2>		percentage in oil phase			:			96.5	99.0		0	100	10.0
		percentage in aqueous phase			:			3.50	1.00		100	0	90.0
		23	77.6	1.00	l	1836	0	1117	5.45	0	0	714	0.105
		24	77.6	1.00	l	102		40.5	0.0551		60.6	0	0.946
Waste		24a	25.0	1.00	l	-102	0	-40.5	-0.0551	0	-60.6	0	-0.946
		28	77.6	1.00	l	1836	0	1117	5.45	0	0	714	0.105
Input		25	25.0	1.00	l	60.6					60.6		
		26	25.0	1.00	l	60.6					60.6		
		27	70.0	1.00	l	60.6					60.6		
		29	75.8	1.00	l	1897	0	1117	5.45	0	60.6	714	0.105
l/l sep <3>		percentage in oil phase			:			96.5	99.0		0	100	10.0
		percentage in aqueous phase			:			3.50	1.00		100	0	90.0
		30	75.8	1.00	l	1797	0	1078	5.40	0	0	714	0.0105
	0.899	31	75.8	1.00	l	99.8		39.1	0.0545		60.6	0	0.0946
Waste		31a	25.0	1.00	l	-99.8	0	-39.1	-0.0545	0	-60.6	0	-0.0946
		32	75.8	1.00	l	1797	0	1078	5.40	0	0	714	0.0105
	Input	34	25.0	1.00	l	1797	0	1078	5.40	0	0	714	0.0105
<s> filter <l>		solubility in solvent (g / g solvent)			:			1.00E-03	1.00E-04		0.0820	100	2.41E-03
		35-A	25.0	1.00	l	715	0	0.714	0.0714	0	0	714	0.0105
		36-A	25.0	1.00	l	1083	0	1077	5.33	0	0	0	0
	Toluene	is the solvent											
	0.0100	g liquid / g solid in sediment											
	48.0	% of liquid phase exits in solid stream											
	Liquid Out	35	25.0	1.00	l	372	0	0.371	0.0371	0	0	371	5.46E-03
Feed		40	25.0	1.00	l	372	0	0.371	0.0371	0	0	371	5.46E-03

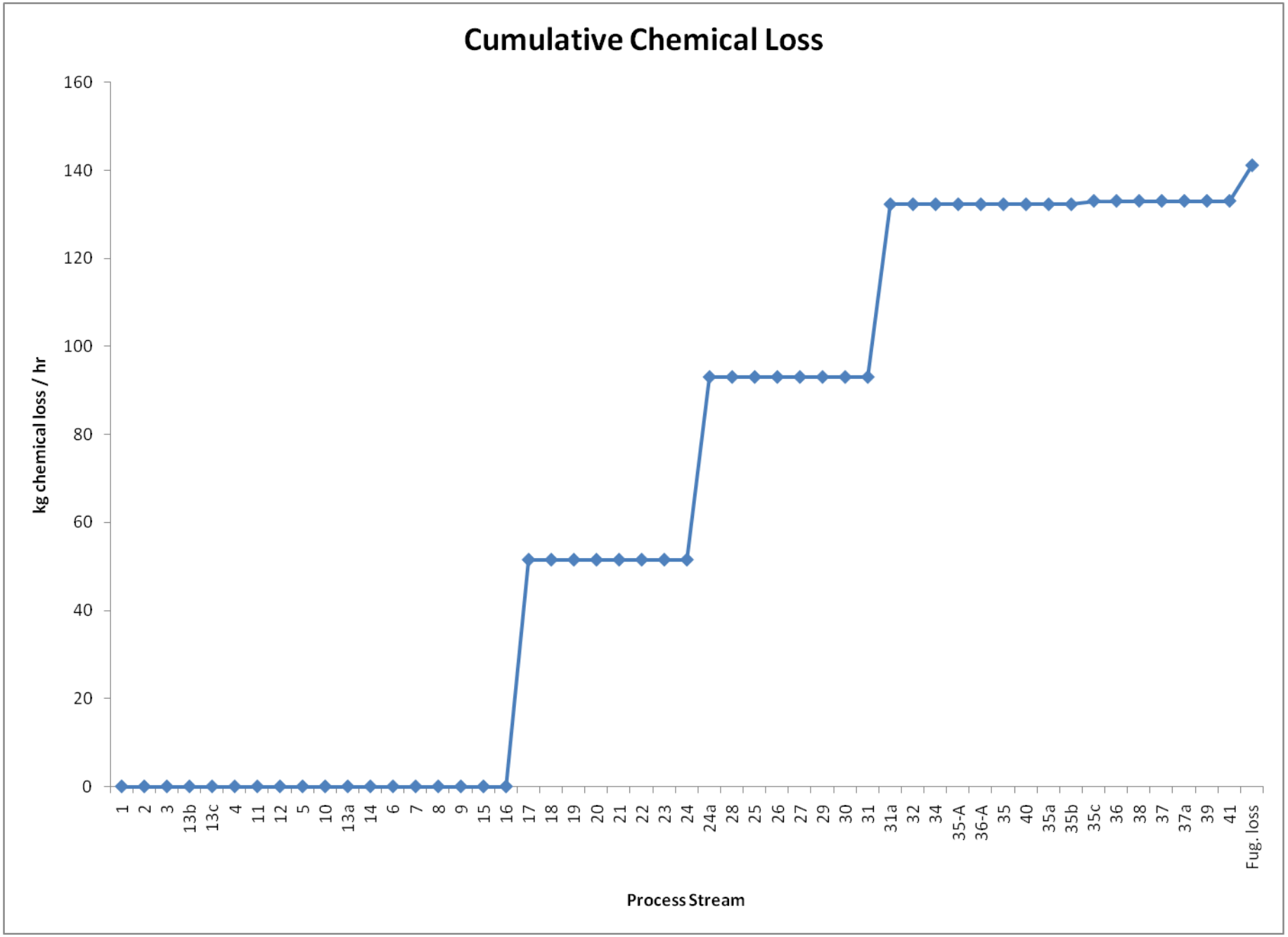
	Comments	Streams	Temp [C]	P	Phase	Total Flow	CDOP	HPPA	DOPO	Hydrogen chloride	Water	Toluene	Zinc chloride
Di <1>		percentage of input in distillate			:			5.00	2.00			99.9	0
		percentage of input in bottoms			:		100	95.0	98.0	100	100	0.1000	100
		Boiling Temperature (Tb) [oC]			:			180	200			111	NA
	Distillate	35a	111	1.00	l	371	0	0.0186	7.42E-04	0	0	371	0
	Bottoms	35b	111	1.00	l	0.766	0	0.353	0.0364	0	0	0.371	5.46E-03
Waste		35c	25.0	1.00	l	-0.766	0	-0.353	-0.0364	0	0	-0.371	-5.46E-03
	Solid Out	36	25.0	1.00	s	1426	0	1078	5.36	0	0	343	5.04E-03
R2	1078	kg	HPPA		:	is converted in rxn (100 % of reactor input)							
		Input to reactor			:	1426	0	1078	5.36	0	0	343	5.04E-03
		R2 Reaction Coefficient 1			:			-1.00	1.00		1.00		
		R2 Conversion 1 [kg/hr]			:	0		-1078	995		82.9		
		R2 Conversion 1 [kgmol/hr]			:	4.60		-4.60	4.60		4.60		
		Flow out of reactor			:	1426	0	0	1000	0	82.9	343	5.04E-03
		Primary product			:	DOPO							
		Total conversion			:		-0	NA	NA	NA	-14.9	-0	-0
		Per pass conversion			:			100	NA		NA	-0	-0
		Total yield from reactor			:			100.0	NA		NA		
	5.04E-06	38	140	0.130	s	1000			1000				5.04E-03
		37	140	0.130	g	426					82.9	343	
		37a	25.0	1.00	l	426	0	0	0	0	82.9	343	0
		39	50.0	1.00	s	1000			1000	0	0	0	5.04E-03
Main product		41	25.0	1.00	s	-1000	0	0	-1000	0	0	0	-5.04E-03
									s				s

	Comments	Streams	Temp [C]	P	Phase	Total Flow	CDOP	HPPA	DOPO	Hydrogen chloride	Water	Toluene	Zinc chloride
		Product purity (%)			:	1.000							
		Main product			:	DOPO							
		Overall Rxn coefficients			:		-1.00		1.00	1.00	-1.00		
		Total yield of process (from reactant)			:		89.9		NA	NA	15.0		
Waste		Fugitive Losses (Total)			g	-8.08	0	0	0	-0.940	0	-7.14	0
		Input Sum			:	1775	1208	0	0	0	556	0.785	10.5
		Fugitive Replacement of Reactants			:	0	0				0		
		Total Input (Input + Fugitive Replacement)			:	1775	1208	0	0	0	556	0.785	10.5
		Product Sum			:	1501	0	0	1000	188	313	0	5.04E-03
		Main product flow			:	1000	0	0	1000	0	0	0	5.04E-03
		Net Input (in - out, omitting fugitives)			:	0.405							

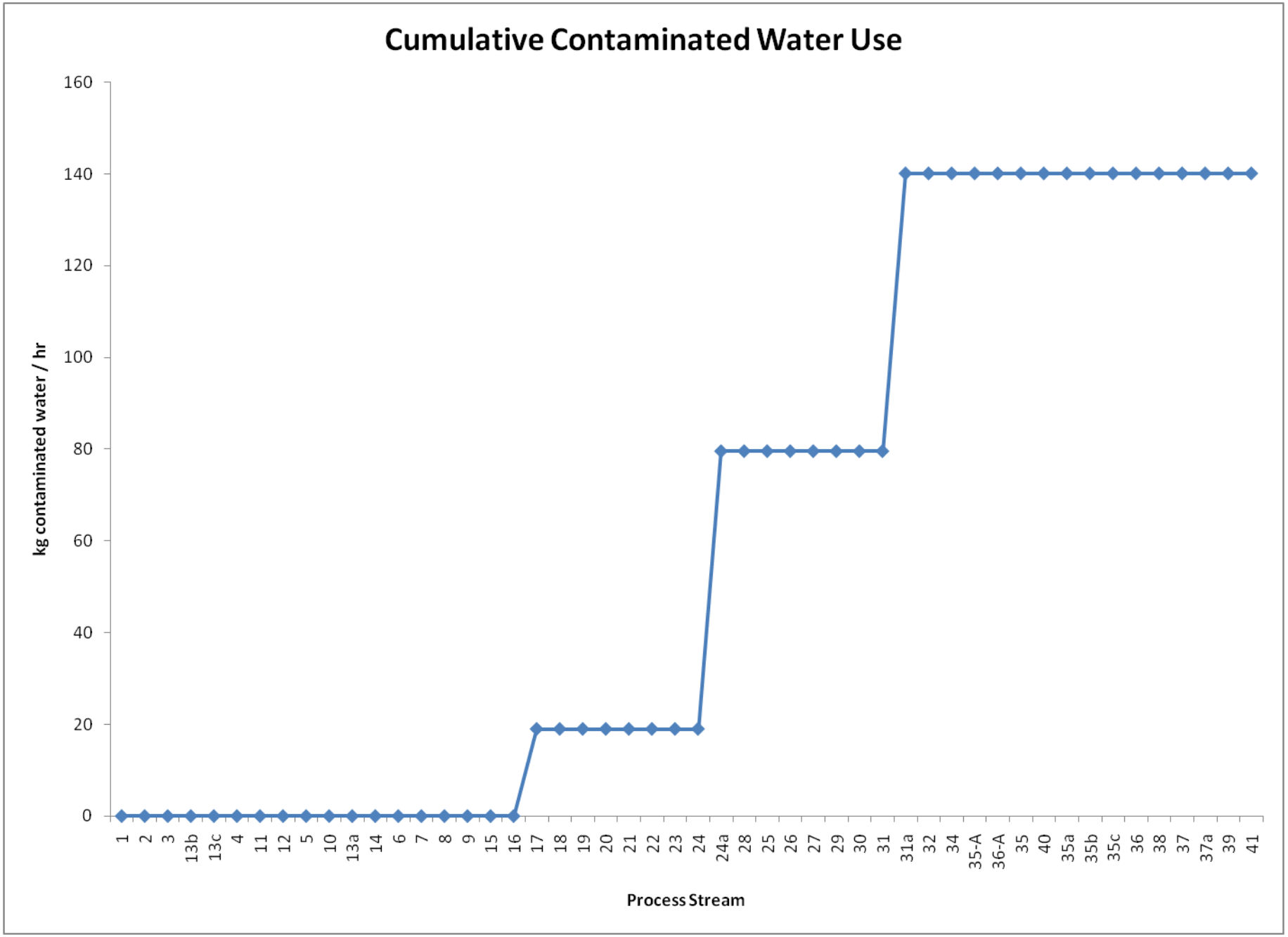
Type		Label	Temp, C	P, atm	Phase	Total flow								Steam	Water
Input		C1	20.0	1.00	l	1574									1574
Cooling out		C2	50.0	1.00	l	-1574									-1574
Input		C3	20.0	1.00	l	1630									1630
Steam out		C4	50.0	1.00	l	-1630									-1630
Input		C5	20.0	1.00	l	86.5									86.5
Steam out		C6	50.0	1.00	l	-86.5									-86.5
Input		C7	20.0	1.00	l	912									912
Cooling out		C8	50.0	1.00	l	-912									-912
Input		C9	20.0	1.00	l	2989									2989
Steam out		C10	50.0	1.00	l	-2989									-2989
Input		C11	20.0	1.00	l	810									810
Steam out		C12	50.0	1.00	l	-810									-810

Input		C13	20.0	1.00	l	0.844									0.844
Steam out		C14	50.0	1.00	l	-0.844									-0.844
Input		S1	207	1.00	l	7.02								7.02	
Steam out		S2	207	1.00	l	-7.02								-7.02	
Input		S3	207	1.00	l	7.02								7.02	
Steam out		S4	207	1.00	l	-7.02								-7.02	
Input		S5	207	1.00	l	463								463	
Steam out		S6	207	1.00	l	-463								-463	
Input		S7	207	1.00	l	116								116	
Steam out		S8	207	1.00	l	-116								-116	

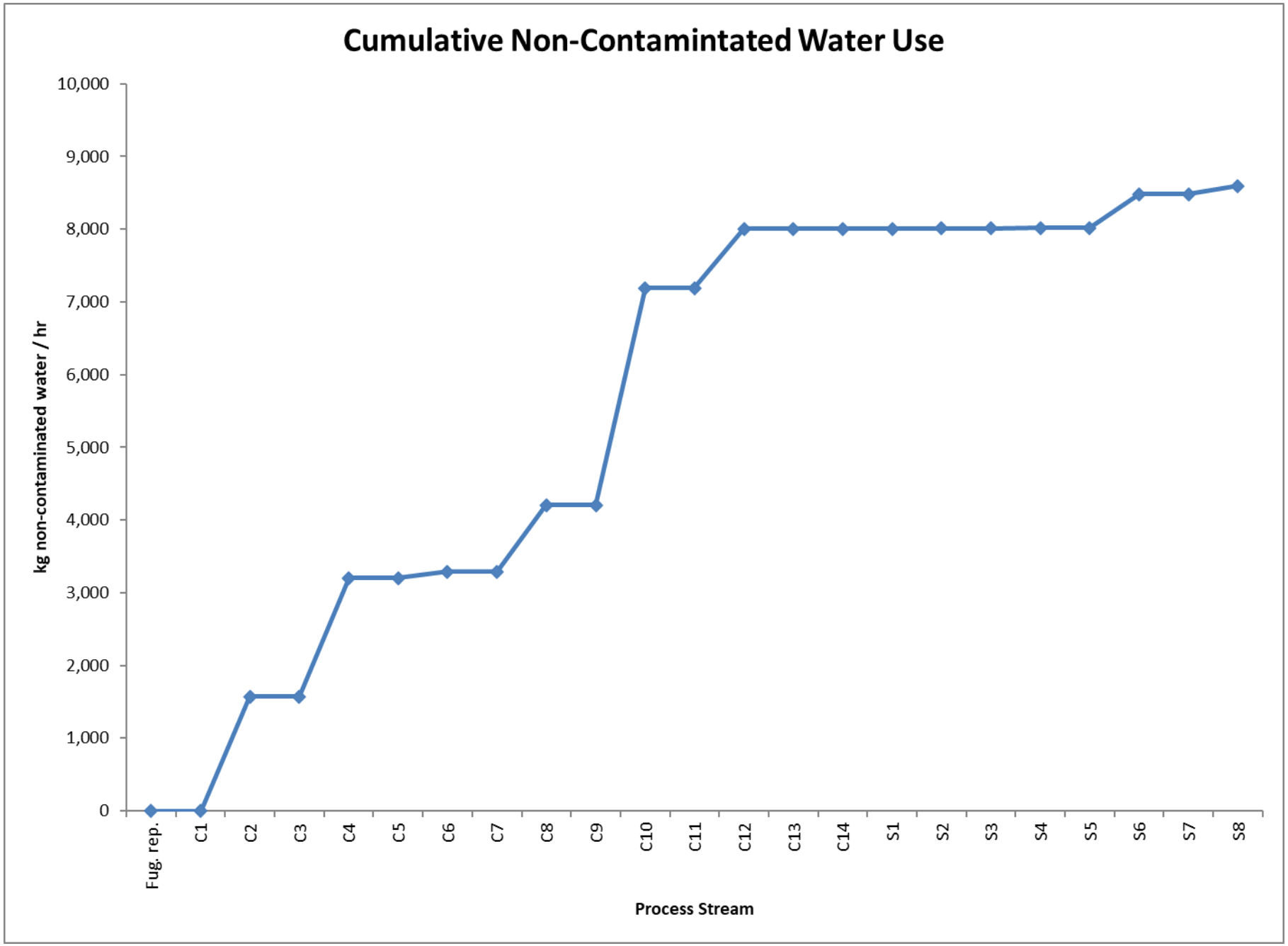
Graph of Cumulative Chemical Losses through Manufacturing Process



Graph of Cumulative Contaminated Water Use / Emission through Manufacturing Process



Graph of Cumulative Non-Contaminated Water Use / Emission through Manufacturing Process



Energy Input for each Unit Process, Cumulative Energy Requirements, Cooling Requirements (exotherms), and Assumed Heat Recovery from Hot Streams Receiving Cooling

Energy Input [MJ / hr]						Cooling Requirements [MJ / hr]							
Process Diagram Label	Unit	Energy input [MJ / 1000 kg Product]	Cumulative energy [MJ / 1000 kg Product]	To [C] (Used to determine energy type)	Energy Type	Process diagram label	Unit	Energy Loss	Cumulative cooling water energy	Tef [C] (for recovery efficiency)	Recovery Efficiency	Energy Recovered	Cumulative recovered [MJ / 1000 kg Product]
P1	Pump 1	1.33E-05	1.33E-05		E	R1	Reactor 1	-232	-232	80.0	0.250	-58.1	-58.1
P2	Pump 2	1.33E-05	2.66E-05		E	Hx4	Heat exchanger 4	-241	-473	96.4	0.250	-60.2	-118
MxE1	Mixer electricity 1	0.409	0.409		E	Hx5	Heat exchanger 5	-12.8	-486	111	0.250	-3.19	-122
P3	Pump 3	1.33E-05	0.409		E	Di1	Distillation condenser 1	-135	-621	110	0.250	-33.7	-155
P4	Pump 4	9.63E-06	0.409		E	Hx7	Heat exchanger 7	-441	-1062	140	0.250	-110	-266
P5	Pump 5	1.06E-06	0.409		E	Hx3	Heat exchanger 3	-120	-1182	75.8	0.250	-29.9	-295
R2	Reactor 2	753	754	140	S	Hx6	Heat exchanger 6	-0.125	-1182	111	0.250	-0.0312	-295
P6	Pump 6	1.73E-03	754		E								
P7	Pump 7	3.50E-03	754		E								
Hx1	Heat exchanger 1	11.4	765	70.0	S								
P8	Pump 8	1.63E-03	765		E								
P9	Pump 9	3.50E-03	765		E								
Hx2	Heat exchanger 2	11.4	776	70.0	S								
MxE2	Mixer electricity 2	0.386	777		E								
MxE3	Mixer electricity 3	0.376	777		E								
Vac1	Vacuum electricity 1	23.8	801		E								
Di1	Distillation reboiler 1	188	989	110	S								

P10	Pump 10	2.40E-05	989		E								
Fk1	Flake 1	67.1	1057	0	E								
	Potential recovery	-295	761										
	Net energy		761				Potential recovery:						-295
	Electricity	92.1	E	[MJ/hr]									
	DowTherm	0	D	[MJ/hr]									
	Heating steam	964	S	[MJ/hr]									
	Direct fuel use	0	F	[MJ/hr]									
	Heating natural gas	0	G	[MJ/hr]									
	Diesel process	0	Ds	[MJ/hr]									
	Undefined	0	U	[MJ/hr]									
	Heating coal	0	C	[MJ/hr]									
	Energy input requirement	1057		[MJ/hr]									
	Cooling water	-1182		[MJ/hr]									
	Cooling refrigeration			[MJ/hr]									
	Potential heat recovery	-295		[MJ/hr]									
	Net energy	761		[MJ/hr]									

Graph of Cumulative Energy Requirements