Reviewed by Michael Overcash 11-4-16
Rereviewed by Michael Overcash 11-8-16 Final

alpha-Methylstyrene as a byproduct of acetone and phenol production [98-83-9]

CONTENTS OF FACTORY GATE TO FACTORY GATE

LIFE CYCLE INVENTORY SUMMARY

Authors	E. Vozzola
Peer reviews, name (date)	Reviewed by MR Overcash on 11-8-2016: route, stoichiometry, and calculations reviewed and found to be representative.
Gtg report last modified on	11-8-2016
Additional notes	

Checked for database consistency on	11-8-2016
First gtg version finalized on	11-8-2016
Modification history, Author (date)	EMV (11-8-2016)

Products	Acetone, Phenol, acetophenone, alpha-methylstyrene
Standard inputs	cumene, Air

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.

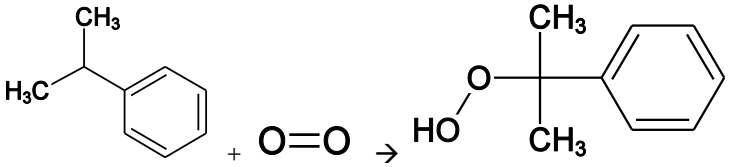
Terms of use: Environmental Clarity does not assume any liability due to use of these lci data. Integration of these data with lci data based on other methodologies is the responsibility of the user. Each report may be updated to improve model accuracy or representativeness.

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

Chemistry

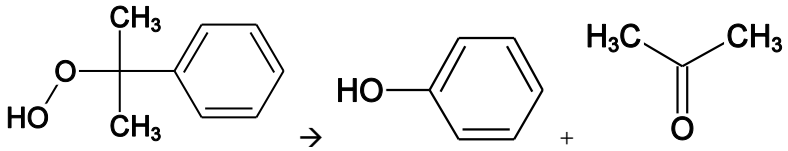
Primary reaction:

$C_6H_5CH(CH_3)_2 + O_2 \rightarrow C_6H_5COOH(CH_3)_2$ (1)



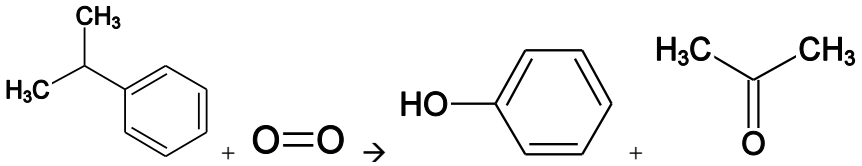
Cumene + Oxygen → Cumene Hydroperoxide

$C_6H_5COOH(CH_3)_2 \rightarrow C_6H_5OH + (CH_3)_2CO$ (2)



Cumene Hydroperoxide → Phenol + Acetone

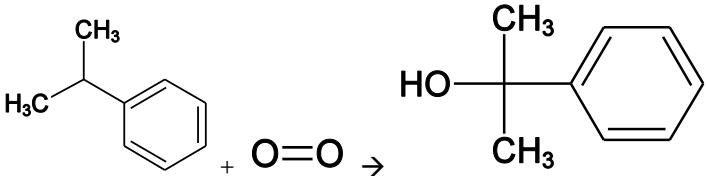
Net reaction: $C_6H_5CH(CH_3)_2 + O_2 \rightarrow C_6H_5OH + (CH_3)_2CO$ (3)



Cumene + Oxygen → Phenol + Acetone

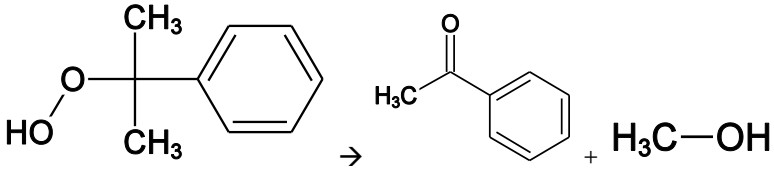
Side reactions: (type of side rxns)

$2\ C_6H_5CH(CH_3)_2 + O_2 \rightarrow 2\ C_6H_5COH(CH_3)_2$ (4)



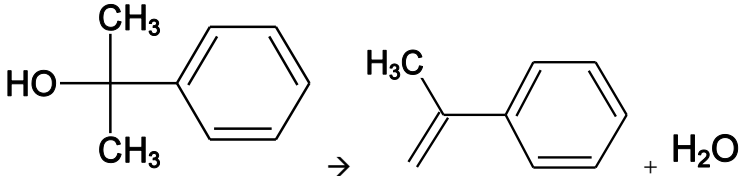
Cumene + Oxygen → a,a-dimethylbenzyl alcohol (DMBA)

$C_6H_5COOH(CH_3)_2 \rightarrow C_6H_5COCH_3 + CH_3OH$ (5)



Cumene Hydroperoxide → Acetophenone + Methanol

$C_6H_5COH(CH_3)_2 \rightarrow C_6H_5C(CH_2)CH_3 + H_2O$ (6)



DMBA → a-Methylstyrene + Water

Notes:

Process Summary

Literature

Note: This gate-to-gate life cycle inventory (gtg lci) shows production of alpha-methylstyrene (AMS) as a byproduct of acetone and phenol production. AMS is formed in Reactor 2, separated and purified as a byproduct. This gtg lci should not be used as the default route to acetone, phenol, or acetophenone because AMS is typically converted back to cumene and recycled, see GTGID 67-64-1.

Approximately 83% of the acetone produced worldwide is manufactured from cumene as a coproduct with phenol [Acetone, Ullmann's]. Cumene Hydroperoxide Process for Phenol and Acetone: Benzene is alkylated to cumene, and then is oxidized to cumene hydroperoxide (CHP), which in turn is cleaved to phenol and acetone, see Reaction 3 in the Chemistry section above.

One kilogram of phenol production results in ~0.6 kg of acetone or about ~0.40-0.45 kg of acetone per kilogram of cumene used. Besides cumene hydroperoxide, both dimethylbenzyl alcohol (DMBA) and acetophenone are also formed as byproducts during this oxidation.

Table 1. Reaction conditions

	KO-Acetone	SRI and Hercules-Ullmann's	Allied/UOP-Ullmann's	Ullmann's Phenol	This Design
Temperature (C)	80-130	90-120	80-100	80-120	100 C
Pressure		4.5-6 bar	1 atm	1-7atm	6 atm
Yield	90-95%	94%			94%
CHP Conc	20-40%			20-40%	25%
Off gas				Cooled to ~ 0C	Cooled to 25 °C to recycle methanol
Selectivity for oxidation		90-94%	92-96%		97%
Heat of oxidation of cumene		-117 kJ/mole			-117 kJ/mole
Heat of cleavage reaction		-252 kJ/mole CH			-252kJ/mole CHP
Selectivity(table 4) for Cleavage		99.5%			100%
Temperature	60-100	<95C	60-80	40-80	80
Reflux		2.8kg acetone/kg cumene hydroperoxide			None

Chemicals Used in this design: Cumene, cumene hydroperoxide, phenol, acetone, sulfur dioxide

Minors: cumylphenols, acetophenone, dimethylbenzyl alcohol (DMBA), alpha-methylstyrene, and hydroxyacetone.

US6225513 give an example of acetone/phenol production that includes by-products and the concentration of each of the components.

SRI-Phenol

Cumene is oxided with air at 103-113 C and 4.4 atm to convert about 20% of the cumene to the hydroperoxide solution. It is then decomposed to phenol and acetone by using sulfuric acid as a catalyst. The phenol and acetone by residual unreacted cumene are separated by distillation. The cumene is recycled

to the reactors. The heavy ends formed are cracked to recover some of the phenol. The yield is 94.3% of theoretical. The process is similar to the BP-Hercules process.

Cumene oxidation – Ullmann's

Fresh and recycled cumene are fed to the reactor, which may operate at 8-12 wt% cumene hydroperoxide. The outlet of stream may contain 25-40 wt% cumene hydroperoxide.

The molar selectivity of the cleavage to phenol and acetone is higher than 99.5% at temperature below 70 C, But it decreases at higher temperature as increasing amounts of DMBA and acetophenone are formed. The reactor temperature is maintained below 95 C by refluxing approximately 2.8 kg acetone per kilogram cumene hydroperoxide.

US7141700

The decomposing vessel is preferably operated at temperature from about 50 C to about 80 C and a pressure from about 115 kPa to about 618 kPa.

Industrial Organic chemistry

$C_6H_5CH(CH_3)_2 + O_2 \rightarrow C_6H_5COOH(CH_3)_2$ $\Delta H = -117\ kJ/mol$

$C_6H_5COOH(CH_3)_2 \rightarrow C_6H_5OH + (CH_3)_2CO$ $\Delta H = -252\ \mathrm{kJ/mole}$

Besides cumene, the water phase is condensed from the off-gas, in which MHP is present. After treatment with diluted caustic soda, the cumene is recycled to the oxidation unit. The water phase is treated at temperature above 100 C and a high pH to decompose the MHP to methanol. Disposal of MHP in the aqueous stream is not allowed since it is toxic to fish.

Caustic soda to remove organic acids and traces of phenol.

Cumene Process – KO

Cumene processes consist of two fundamental chemical reactions: cumene is oxidized with air to form cumene hydroperoxide, and cumene hydroperoxide is cleaved to yield phenol and acetone. In this process, approximately 0.46 kg of acetone and 0.75 kg of phenol are produced per kg of cumene feedstock. The overall yield for the cumene process is 96 mol %.

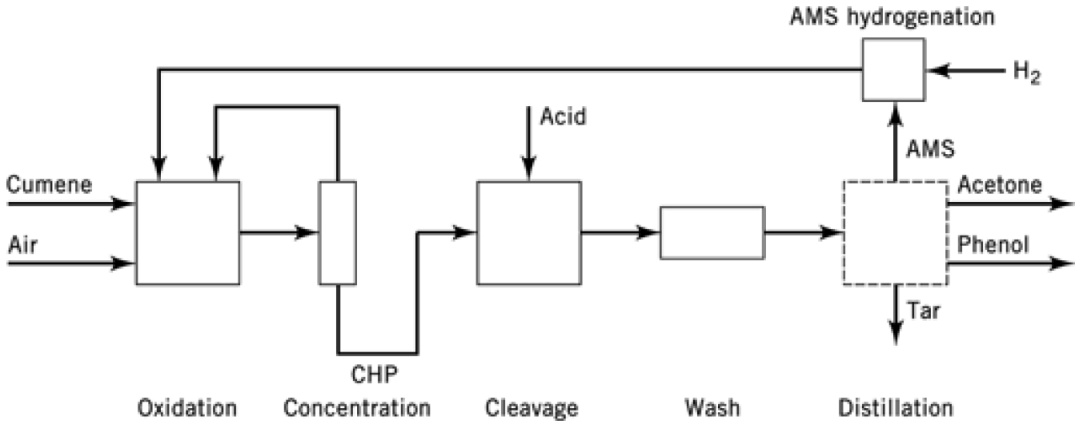


Fig. 1. Cumene process for phenol production.

Table 2. Chemicals Used in design

Chemical Name	CAS	Formula	Short Name
Cumene	98-82-8	C9H12	
Cumene Hydroperoxide	80-15-9	C9H12O2	CHP
Dimethylbenzyl alcohol	617-94-7	C9H12O	DMBA
Formic acid			
Acetic acid			
Methyl Hydroperoxide			MHP – off gas
Methanol			
Acetophenone	98-86-2	C8H8O	ACP
a-methylstyrene	98-83-9	C9H10	AMS
Dicumyl peroxide	80-43-3	C18H22O2	DCP
Phenol	108-95-2		
Acetone	67-64-1		

Acetophenone byproduct – added 2016

Production of acetophenone is satisfied through recovery as a byproduct from phenol and acetone production (Ullmann's, 2000; Kirk Othmer, 2001; Kirk Othmer, 2011). Acetophenone is a colorless liquid with a sweet orange blossom odor. It is used as an intermediate in the production of synthetic resins, pharmaceuticals, and fragrances (Ullmann's, 2000). Phenol and acetone are produced as main products with acetophenone, alpha-methylstyrene, hydroxyacetone, and mesityl oxide produced as byproducts in a process known as the Hock process (Kirk Othmer, 2011). The yield of byproducts varies by manufacturer and can be optimized with adjustments to the inputs. Typical byproduct yields are not readily available in the literature. The yields are likely adjusted frequently to reflect market demand. In this gtg, 1.8% of the cumene hydroperoxide formed reacts to acetophenone.

Acetophenone is isolated from phenol residues via separation methods such as azeotropic distillation (Ullmann's 2000; Kirk Othmer, 2001; WO2009055535 A2). Binary azeotropes of phenol and acetophenone are shown in Table 3.

Table 3. Azeotropes of phenol and acetophenone

P, atm	Phenol b. p., °C	Acetophenone b. p., °C	Azeotrope b. p., °C	Mass fraction acetophenone
0.0658	102.7	115.4	118.3	0.707
0.132	119.7	133.9	135.9	0.725
0.340	146.1	182.7	163.6	0.803
0.680	168.3	184.9	187.2	0.880
1.00	181.9	201.8	201.8	0.939
1.07	184.3	204.4	204.4	0.950
1.34	192.9	213.8	213.8	0.994
1.68	201.8	223.7	--	--
2.02	209.4	232.1	--	--
3.31	232.3	257.4	--	--

This gtg shows vacuum distillation of acetophenone/phenol at 0.132 atm to separate acetophenone from the phenol residue.

Route Review 2016 – with respect to acetophenone production

KO (2001), Ul (2000), and ReachCentrum (2010) consistent with current route.
KO and Ul give four production methods:
1. as a byproduct of phenol manufacture (via cumene hydroperoxide)
2. directly from cumene hydroperoxide
3. ethylbenzene + O2 (selectivity limited to 25%)
4. benzene + O2 (no longer used/not of industrial importance)

Method 1 is shown in this report. KO (2001), Ul (2000), and ReachCentrum 2010 report indicate that world production is met through production as a byproduct of phenol manufacture, Method 1. WO 2009055535 A2 (2009) gives a method for optimizing this production from the phenol process. We conclude that the most representative route is Method 1. Note that acetophenone is also called methyl phenyl ketone.

LCI design

In this design, acetone is produced using the cumene-to-acetone process, but a modification is made to recover AMS. Cumene is oxidized with air to form cumene hydroperoxide (CHP). The peroxide is subsequently decomposed to acetone and phenol using a strong mineral acid as a catalyst. Acetophenone and AMS are produced as byproducts.

The cumene oxidation reactor operates at 100 °C and 6 atm. The reaction is exothermic with a heat of reaction of -117 kJ/mole. The final CHP concentration is about 25% with the balance being reactants. In this oxidation process, dimethylbenzyl alcohol (DMBA) and acetophenone (ACP) is formed as by-products. The off-gas from the reactors is cooled to recycle the methanol, which is a byproduct of acetophenone reaction, and cumene back to the reactor. The product from the oxidation unit is concentrated to about 90 wt% CHP with vacuum distillation, the so-called concentration unit, at 0.2 atm. Cumene is separated and recycled back to the reactor. The concentrated CHP is sent to cleavage reactor and decompose into acetone and phenol (using sulfuric acid, about 0.01 kg/kg phenol or 0.007 kg/kg cumene), which is an exothermic process with a heat of reaction of -252 kJ/mole. The neutralized material is sent to recovery unit to get acetone and phenol. The a-methylstyrene is recovered from distillation column 3 and purified in distillation column 3a and distillation column 3b. The overhead from distillation column 3a contains primarily cumene and is recycled to the reactor. The overhead from column 3b contains 99.7% pure AMS and is cooled to 25 °C at 1 atm and sent as the main product of this gtg lci. The bottoms from distillation column 3b contain phenol and are sent as a byproduct. The bottoms from distillation column 4 are vacuum distilled at 0.13 atm to recover acetophenone as a byproduct.

Note: In practice, the product from the cleavage reactor (R2) is neutralized using sodium hydroxide (about 0.01 kg/kg phenol or 0.007 kg/kg cumene input), to separate the sulfuric acid used as catalyst and the formic and acetic acids formed as byproducts in the reactor. The sulfuric acid catalyst and formic and acetic acid byproducts are not shown in this gtg due to small amounts used/formed. Thus, the subsequent neutralization is also not shown.

References

Engenharia Quimica, Cumune oxidation to cumene hydroperoxide, University of Tecnica de Lisboa

Kirk Othmer (2001), Kirk Othmer Encyclopedia of Chemical Technology, Ketones (Y.-L. Hwang and T. C. Bedard)

Kirk Othmer (2010), Kirk Othmer Encyclopedia of Chemical Technology, Phenol (Jim Wallace, M.W. Kellogg Company)

Kirk Othmer (2010, 2011), Kirk Othmer Encyclopedia of Chemical Technology, Acetone (William L. Howard, the Dow Chemical Company)

Ullmann's (2000), Ullmann's Encyclopedia of Industrial Chemistry, Ketones (H. Seigel and M. Eggersdorfer)

Ullmann's (2010), Ullmann's Encyclopedia of Industrial Chemistry, Acetone (Stylianos Sifniades, and Alan B. Levy)

Ullmann's (2010), Ullmann's Encyclopedia of Industrial Chemistry, Phenol (Manfred Weber, Markus Weber, and Michael Kleine-Boymann)

WO2009055535 A2 (2009) recovery of acetophenone during the production of phenol (J. R. Black, L. W. Payne, P. E. Unger)

Critical parameters

Conversion / Yield information from both reactors			
		Conversion of or Yield from Cumene	Conversion of or Yield from CHP
Total conversion in reactor 1: (% of reactant entering the process that reacts)	From mass balance	99.8%	
Total per pass conversion in reactor 1: (% of reactant entering the reactor that reacts)	From mass balance	19.6%	
Total yield of reactor 1: (% yield cumene peroxide produced in the reactor based on reactant input to process)	From mass balance	92.2%	
Total conversion in reactor 2: (% of reactant entering the process that reacts)	From mass balance		NA
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	6%	
Notes: Total yield of process from cumene with respect to AMS is 6%. The yield from cumene for all products (phenol, acetone, acetophenone and AMS) is >90%.			

Product purity		
	AMS	Comments
Used here	99.7%	

Summary of LCI Information

Standard inputs					
UID	Name	Flow	Purity	Units	Comments
98-82-8	Cumene	1.66E+04	-	[kg/hr]	
UIDAir	Air	1.84E+04	-	[kg/hr]	
	Total	3.50E+04		[kg/hr]	
Non-reacting inputs					
UID	Name	Flow	Purity	Units	Comments
	Total	0		[kg/hr]	
Ancillary inputs					
UID	Name	Flow	Purity	Units	Comments
	Total	0		[kg/hr]	
Products					
UID	Name	Flow	Purity	Units	Comments
67-64-1	Acetone	7430	99.7	[kg/hr]	
108-95-2	Phenol	1.20E+04	99.9	[kg/hr]	
98-86-2	acetophenone	240	100	[kg/hr]	
98-83-9	alpha-methylstyrene	1000	0.997	[kg/hr]	
	Total	2.06E+04		[kg/hr]	
Benign outflows					
UID	Name	Flow	Purity	Units	Comments
7727-37-9	Nitrogen	1.41E+04	-	[kg/hr]	
7732-18-5	Water	119	-	[kg/hr]	
	Total	1.42E+04		[kg/hr]	

Process emissions							
UID	Name	Gas	Liquid	Solid	Solvent	Units	Comments
98-82-8	Cumene	3.40	0	0	0	[kg/hr]	
98-86-2	acetophenone	0	31.2	0	0	[kg/hr]	
108-95-2	Phenol	0	11.8	0	0	[kg/hr]	
67-64-1	Acetone	148	0	0	0	[kg/hr]	
67-56-1	Methanol	82.4	0.732	0	0	[kg/hr]	
	Total	234	43.8	0	0		

Mass balance	
Total inputs	3.50E+04
Total outflows	3.52E+04
Net input	-156

Energy use			
Energy type	Amount	Units	Comments
electricity	5062	[MJ/hr]	Net electricity use at plant
heating steam	8.05E+04	[MJ/hr]	heating by steam (0.85 efficiency included)
Net input requirement	8.56E+04	[MJ/hr]	Net of energies input to system
cooling water	- 1.20E+05	[MJ/hr]	net cooling by cooling water
potential recovery	- 3.73E+04	[MJ/hr]	potential energy recovery (negative)
Net energy	4.83E+04	[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,

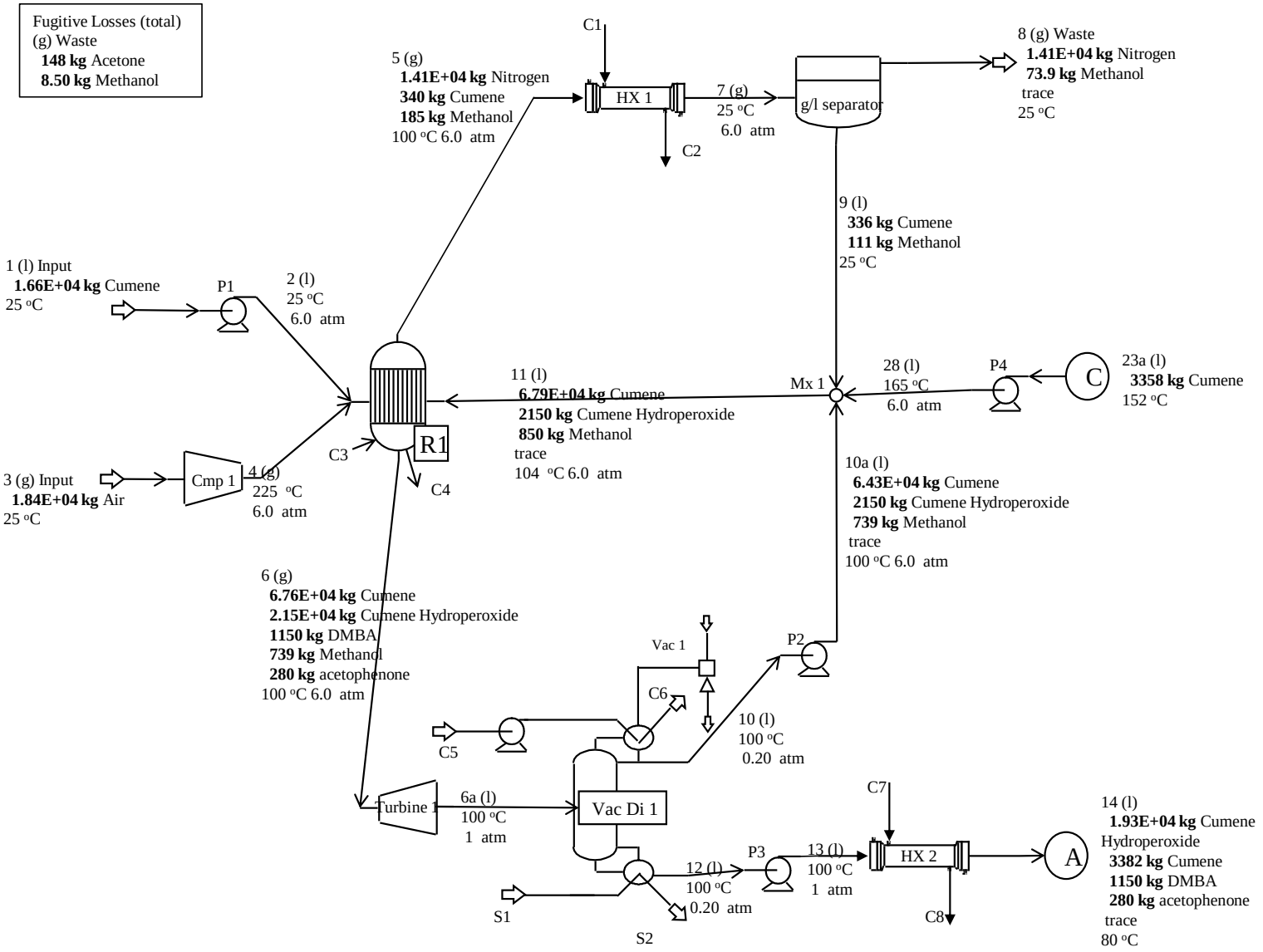
- generally numbers progress from the start to the end of the process
- numbers are used for process streams
- C i , i = 1,..n are used for all cooling non-contact streams
- S j, j = 1,...n are used for all steam heating non-contact streams

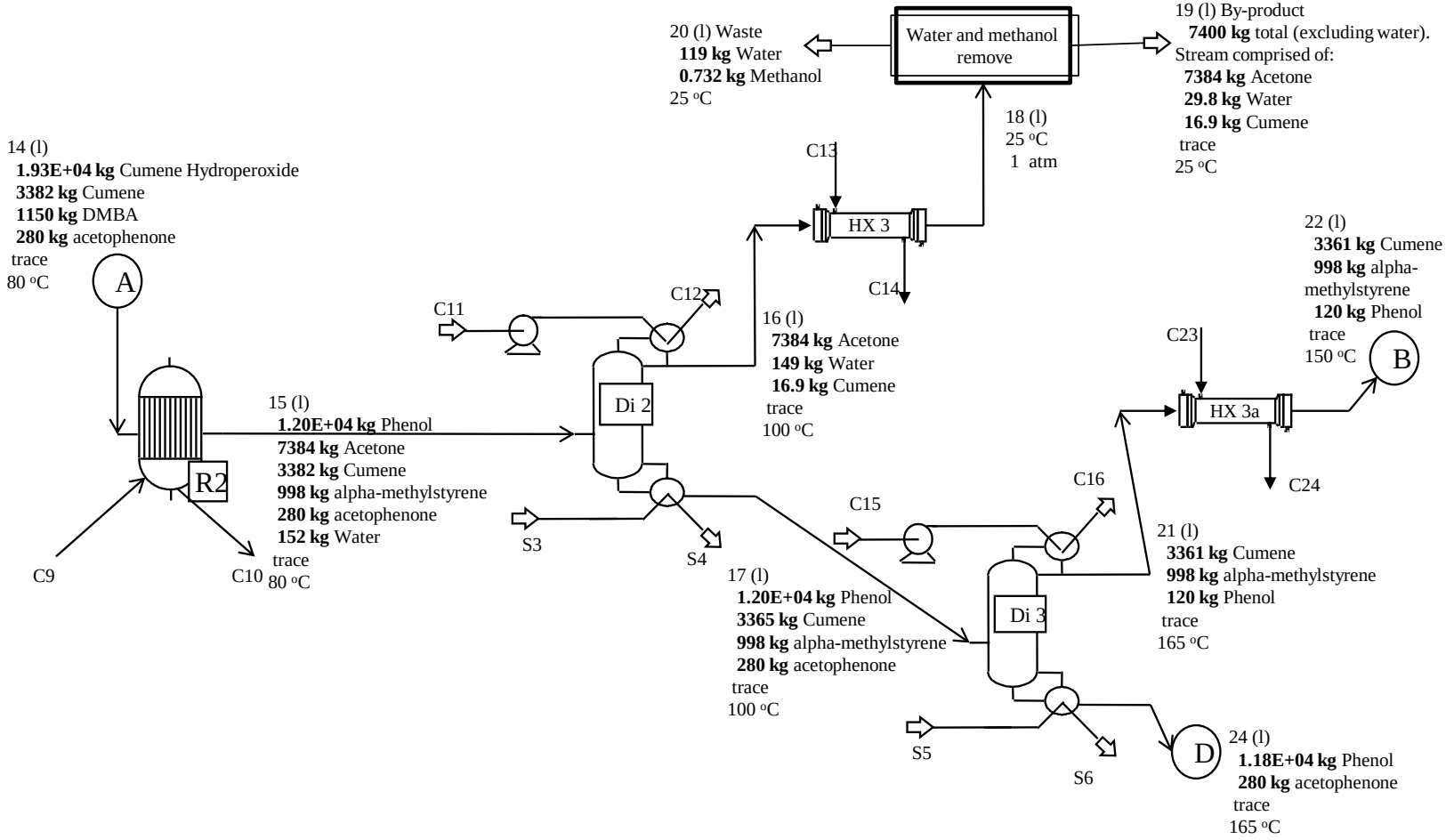
5) Recycle streams are shown with dotted lines

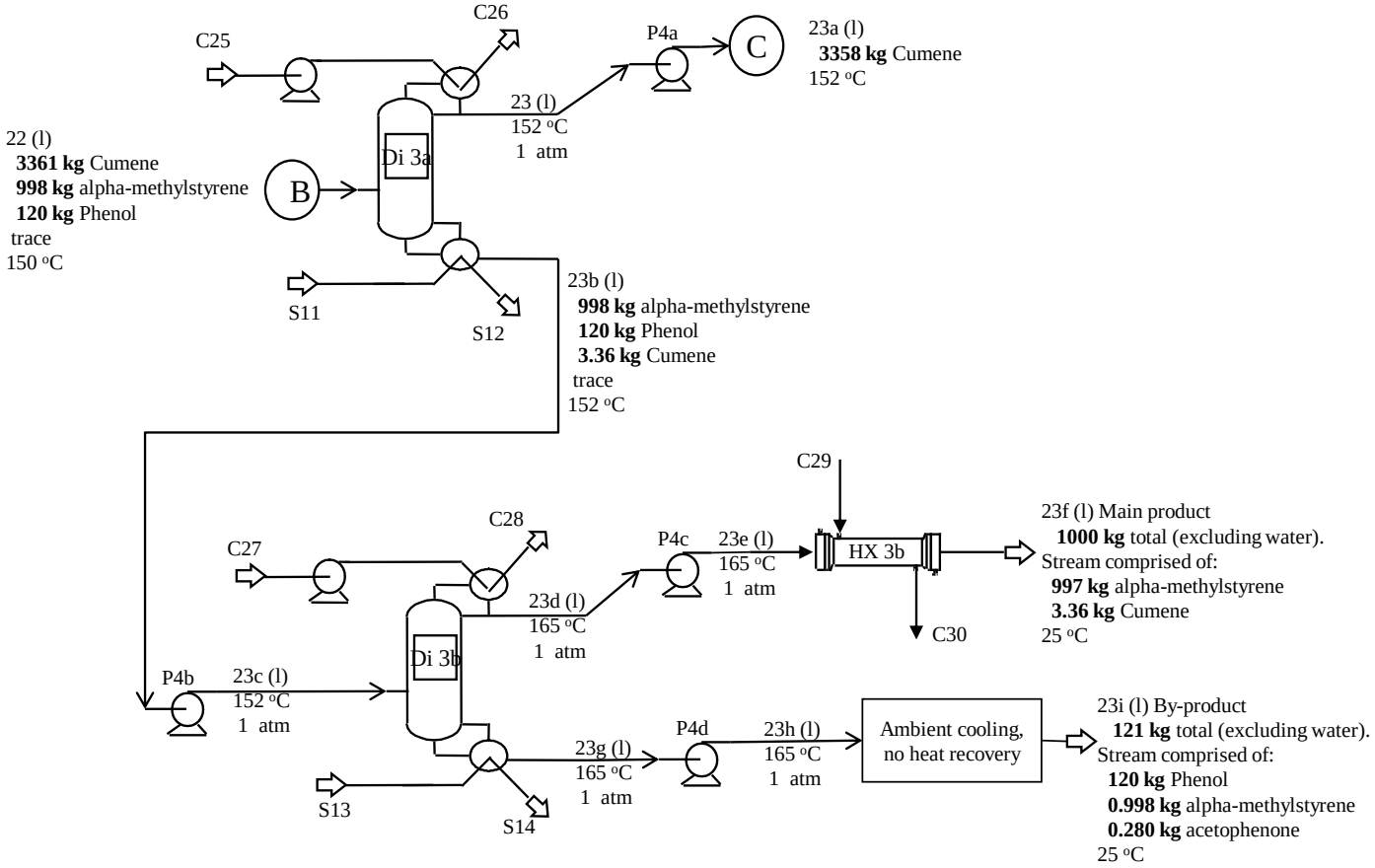
For most streams, the temperature and pressure are shown, if the pressures are greater than 1 atm

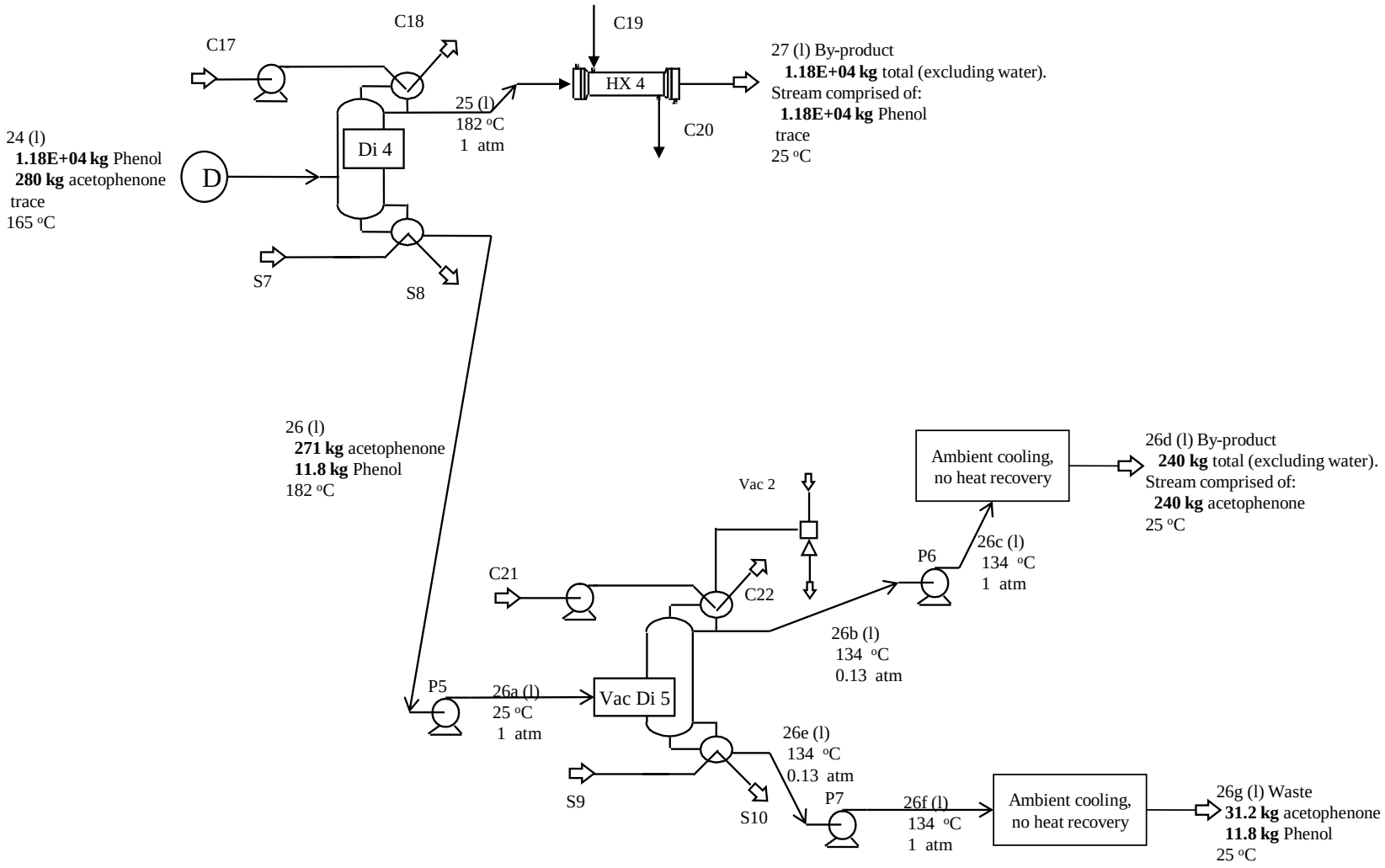
Process Diagram or Boundary of LCI

Steam enters the process as a gas at 207 °C and leaves as a liquid at 207 °C. Cooling water enters at 20 °C and leaves at 50 °C.
Unless otherwise indicated, all processes are at 1 atm and 25 °C.




14 (l)
1.93E+04 kg Cumene Hydroperoxide
3382 kg Cumene
1150 kg DMBA
280 kg acetophenone
trace
80 °C
A
R2
C9
C10
15 (l)
1.20E+04 kg Phenol
7384 kg Acetone
3382 kg Cumene
998 kg alpha-methylstyrene
280 kg acetophenone
152 kg Water
trace
80 °C
C11
Di 2
S3
S4
C12
16 (l)
7384 kg Acetone
149 kg Water
16.9 kg Cumene
trace
100 °C
HX 3
C13
C14
18 (l)
25 °C
1 atm
Water and methanol remove
20 (l) Waste
119 kg Water
0.732 kg Methanol
25 °C
19 (l) By-product
7400 kg total (excluding water).
Stream comprised of:
7384 kg Acetone
29.8 kg Water
16.9 kg Cumene
trace
25 °C
C15
17 (l)
1.20E+04 kg Phenol
3365 kg Cumene
998 kg alpha-methylstyrene
280 kg acetophenone
trace
100 °C
Di 3
S5
S6
C16
21 (l)
3361 kg Cumene
998 kg alpha-methylstyrene
120 kg Phenol
trace
165 °C
C23
HX 3a
C24
22 (l)
3361 kg Cumene
998 kg alpha-methylstyrene
120 kg Phenol
trace
150 °C
B
D
24 (l)
1.18E+04 kg Phenol
280 kg acetophenone
trace
165 °C


C25
C26
P4a
C
23a (l)
3358 kg Cumene
152 °C
23 (l)
152 °C
1 atm
22 (l)
3361 kg Cumene
998 kg alpha-methylstyrene
120 kg Phenol
trace
150 °C
Di 3a
B
S11
S12
23b (l)
998 kg alpha-methylstyrene
120 kg Phenol
3.36 kg Cumene
trace
152 °C
C29
C28
C27
P4c
23e (l)
165 °C
1 atm
HX 3b
23f (l) Main product
1000 kg total (excluding water).
Stream comprised of:
997 kg alpha-methylstyrene
3.36 kg Cumene
25 °C
23d (l)
165 °C
1 atm
C30
Di 3b
P4b
23c (l)
152 °C
1 atm
P4d
23h (l)
165 °C
1 atm
Ambient cooling,
no heat recovery
23g (l)
165 °C
1 atm
23i (l) By-product
121 kg total (excluding water).
Stream comprised of:
120 kg Phenol
0.998 kg alpha-methylstyrene
0.280 kg acetophenone
25 °C
S13
S14


C17
C18
C19
HX 4
C20
27 (l) By-product
1.18E+04 kg total (excluding water).
Stream comprised of:
1.18E+04 kg Phenol
trace
25 °C
25 (l)
182 °C
1 atm
24 (l)
1.18E+04 kg Phenol
280 kg acetophenone
trace
165 °C
D
Di 4
S7
S8
26 (l)
271 kg acetophenone
11.8 kg Phenol
182 °C
Ambient cooling, no heat recovery
26d (l) By-product
240 kg total (excluding water).
Stream comprised of:
240 kg acetophenone
25 °C
Vac 2
C21
C22
P6
26c (l)
134 °C
1 atm
26b (l)
134 °C
0.13 atm
P5
26a (l)
25 °C
1 atm
Vac Di 5
26e (l)
134 °C
0.13 atm
S9
S10
P7
26f (l)
134 °C
1 atm
Ambient cooling, no heat recovery
26g (l) Waste
31.2 kg acetophenone
11.8 kg Phenol
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	Cumene	Cumene Hydroperoxide	DMBA	acetophenone	alpha-methylstyrene	Dicumyl Peroxide	Phenol	Acetone	Air	Nitrogen	Oxygen	Hydrogen	Methanol	Water
Input		1	25.0	1.00	l	1.66E+04	1.66E+04													
		2	25.0	6.00	l	1.66E+04	1.66E+04													
Input		3	25.0	1.00	g	1.84E+04									1.84E+04					
		4	225	6.00	g	1.84E+04										1.41E+04	4284			
		Stream 11:Recycle input				7.09E+04	6.79E+04	2150	0.115	0.0280	0	0	0	0	0	0	0	0	850	0
		Stream 11:Recycle calculated				7.09E+04	6.79E+04	2150	0.115	0.0280	0	0	0	0	0	0	0	0	850	0
		Stream 11:Recycle residue				7.77E-03	1.45E-03	4.72E-05	2.46E-09	5.99E-10	0	0	0	0	0	0	0	0	6.28E-03	0
R1	1.61E+04	kg	Cumene		:	is converted in rxn (19.0 % of reactor input)														
	507	kg	Cumene		:	is converted in rxn (0.600 % of reactor input)														
	355	kg	Cumene Hydroperoxide		:	is converted in rxn (16.5 % of reactor input)														
		Input to reactor			:	1.06E+05	8.45E+04	2150	0.115	0.0280	0	0	0	0	0	1.41E+04	4284	0	850	0
		R1 Reaction Coefficient 1			:		-1.00	1.00									-1.00			
		R1 Conversion 1 [kg/hr]			:	0	-1.61E+04	2.03E+04									-4284			
		R1 Conversion 1 [kgmol/hr]			:	134	-134	134									-134			
		R1 Reaction Coefficient 2			:		-1.00	-1.00	2.00											
		R1 Conversion 2 [kg/hr]			:	0	-507	-643	1150											
		R1 Conversion 2 [kgmol/hr]			:	4.23	-4.23	-4.23	8.45											
		R1 Reaction Coefficient 3			:			-1.00		1.00									1.00	
		R1 Conversion 3 [kg/hr]			:	0		-355		280									74.7	
		R1 Conversion 3 [kgmol/hr]			:	2.33		-2.33		2.33									2.33	
		Flow out of reactor		0.240	:	1.06E+05	6.80E+04	2.15E+04	1150	280	0	0	0	0	0	1.41E+04	0	0	924	0
		Primary product			:	Cumene Hydroperoxide														
		Total conversion			:		99.8	NA	NA	NA	NA	NA	NA	NA	-0	NA	NA	NA	NA	NA
		Per pass conversion			:		19.6	NA	NA	NA						-0	100		NA	
		Total yield from reactor			:		92.2	NA									95.1			
Display in PFD		5	100	6.00	g	1.47E+04	340								0	1.41E+04	0	0	185	
Display in PFD		6	100	6.00	g	9.13E+04	6.76E+04	2.15E+04	1150	280	0	0	0	0	0	0	0	0	739	
		7	25.0	6.00	g	1.47E+04	340	0	0	0	0	0	0	0	0	1.41E+04	0	0	185	
Waste		8	25.0	1.00	g	-1.42E+04	-3.40									-1.41E+04	0		-73.9	
Display in PFD		9	25.0	1.00	l	447	336	0	0	0	0	0	0	0	0	0	0	0	111	0
Feed		6a	100	1.00	l	9.13E+04	6.76E+04	2.15E+04	1150	280	0	0	0	0	0	0	0	0	739	
Di <1>		percentage of input in distillate			:		95.0	10.0	0.0100	0.0100									99.9	
		percentage of input in bottoms			:		5.00	90.0	100.0	100.0	100	100	100	100	100	100	100	100	0.1000	100
		Boiling Temperature (Tb) [oC]			:		152	170	202	202									64.8	
Distillate		10	100	0.200	l	6.71E+04	6.43E+04	2150	0.115	0.0280	0	0	0	0	0	0	0	0	739	0
Bottoms		12	100	0.200	l	2.42E+04	3382	1.93E+04	1150	280	0	0	0	0	0	0	0	0	0.739	0
Display in PFD		10a	100	6.00	l	6.71E+04	6.43E+04	2150	0.115	0.0280	0	0	0	0	0	0	0	0	739	
Display in PFD		11	104	6.00	l	7.09E+04	6.79E+04	2150	0.115	0.0280	0	0	0	0	0	0	0	0	850	0
		13	100	1.00	l	2.42E+04	3382	1.93E+04	1150	280	0	0	0	0	0	0	0	0	0.739	0
Display in PFD		14	80.0	1.00	l	2.42E+04	3382	1.93E+04	1150	280	0	0	0	0	0	0	0	0	0.739	

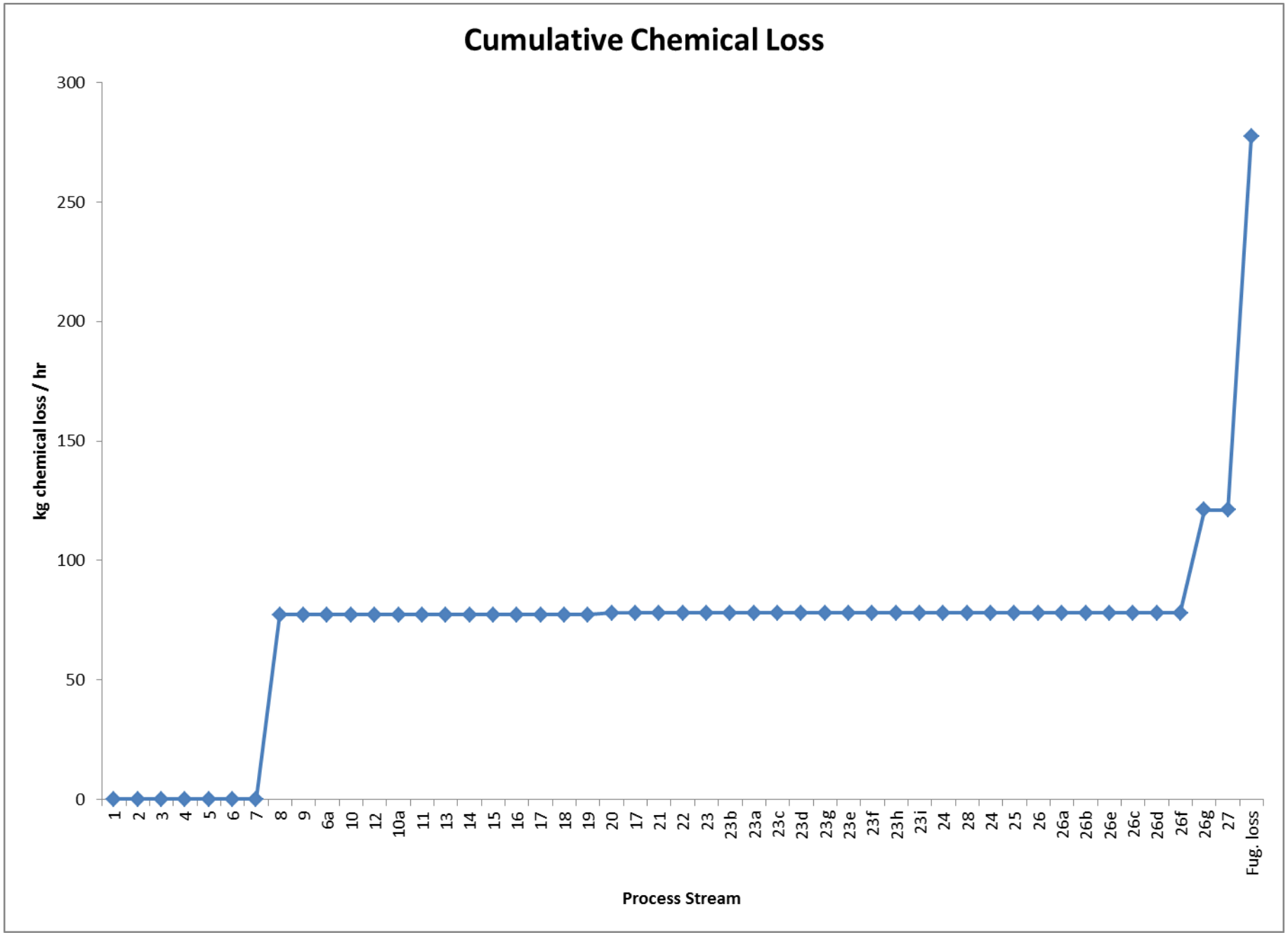
	Comments	Streams	Temp [C]	P	Phase	Total Flow	Cumene	Cumene Hydroperoxide	DMBA	acetophenone	alpha-methylstyrene	Dicumyl Peroxide	Phenol	Acetone	Air	Nitrogen	Oxygen	Hydrogen	Methanol	Water
R2	1.93E+04	kg	Cumene Hydroperoxide		:	is converted in rxn (100 % of reactor input)														
	1150	kg	DMBA		:	is converted in rxn (100 % of reactor input)														
		Input to reactor			:	2.42E+04	3382	1.93E+04	1150	280	0	0	0	0	0	0	0	0	0.739	
		R2 Reaction Coefficient 1			:			-1.00					1.00	1.00						
		R2 Conversion 1 [kg/hr]			:	0		-1.93E+04					1.20E+04	7384						
		R2 Conversion 1 [kgmol/hr]			:	127		-127					127	127						
		R2 Reaction Coefficient 2			:				-1.00		1.00									1.00
		R2 Conversion 2 [kg/hr]			:	0			-1150		998									152
		R2 Conversion 2 [kgmol/hr]			:	8.45			-8.45		8.45									8.45
		Flow out of reactor			:	2.42E+04	3382	0	0	280	998	0	1.20E+04	7384	0	0	0	0	0.739	152
		Primary product			:	Acetone														
		Total conversion			:		-0	NA	NA	NA	NA	NA	NA	NA	-0	NA	NA	NA	NA	NA
		Per pass conversion			:		-0	100	100	-0	NA		NA	NA					-0	NA
		Total yield from reactor			:			100					NA	NA						
Display in PFD	Feed	15	80.0	1.00	l	2.42E+04	3382	0	0	280	998	0	1.20E+04	7384	0	0	0	0	0.739	152
Di <2>		percentage of input in distillate			:		0.500	0	0	0	0	0	0	100					100	98.0
		percentage of input in bottoms			:		99.5	100	100	100	100	100	100	0	100	100	100	100	0	2.00
		Boiling Temperature (Tb) [oC]			:		152			202	165		182	56.3					64.8	100
Display in PFD	Distillate	16	100	1.00	l	7550	16.9	0	0	0	0	0	0	7384	0	0	0	0	0.739	149
Display in PFD	Bottoms	17	100	1.00	l	1.66E+04	3365	0	0	280	998	0	1.20E+04	0	0	0	0	0	0	3.04
		18	25.0	1.00	l	7550	16.9	0	0	0	0	0	0	7384	0	0	0	0	0.739	149
By-product		19	25.0	1.00	l	-7430	-16.9							-7384					-7.39E-03	-29.8
Waste		20	25.0	1.00	l	-120	0	0	0	0	0	0	0	0	0	0	0	0	-0.732	-119
Display in PFD	Feed	17	100	1.00	l	1.66E+04	3365	0	0	280	998	0	1.20E+04	0	0	0	0	0	0	3.04
Di <3>		percentage of input in distillate			:		99.9			0.100	100		1.00							
		percentage of input in bottoms			:		0.1000	100	100	99.9	0	100	99.0	100	100	100	100	100	100	100
		Boiling Temperature (Tb) [oC]			:		152			203	165		182							100
Display in PFD	Distillate	21	165	1.00	l	4479	3361	0	0	0.280	998	0	120	0	0	0	0	0	0	0
Display in PFD	Feed	22	150	1.00	l	4479	3361	0	0	0.280	998	0	120	0	0	0	0	0	0	0
Di <3a>		percentage of input in distillate			:		99.9			0	0		0							
		percentage of input in bottoms			:		0.1000	100	100	100	100	100	100	100	100	100	100	100	100	100
		Boiling Temperature (Tb) [oC]			:		152			202	165		182							
	Distillate	23	152	1.00	l	3358	3358	0	0	0	0	0	0	0	0	0	0	0	0	0
Display in PFD	Bottoms	23b	152	1.00	l	1121	3.36	0	0	0.280	998	0	120	0	0	0	0	0	0	0
Display in PFD		23a	152	1.00	l	3358	3358	0	0	0	0	0	0	0	0	0	0	0	0	0
	Feed	23c	152	1.00	l	1121	3.36	0	0	0.280	998	0	120	0	0	0	0	0	0	0
Di <3b>		percentage of input in distillate			:		100			0	99.9		0							
		percentage of input in bottoms			:		0	100	100	100	0.1000	100	100	100	100	100	100	100	100	100
		Boiling Temperature (Tb) [oC]			:		152			202	165		182							
	Distillate	23d	165	1.00	l	1000	3.36	0	0	0	997	0	0	0	0	0	0	0	0	0
	Bottoms	23g	165	1.00	l	121	0	0	0	0.280	0.998	0	120	0	0	0	0	0	0	0
		23e	165	1.00	l	1000	3.36	0	0	0	997	0	0	0	0	0	0	0	0	0
Main product		23f	25.0	1.00	l	-1000	-3.36	0	0	0	-997	0	0	0	0	0	0	0	0	0
		23h	165	1.00	l	121	0	0	0	0.280	0.998	0	120	0	0	0	0	0	0	0
By-product		23i	25.0	1.00	l	-121	0	0	0	-0.280	-0.998	0	-120	0	0	0	0	0	0	0
Display in PFD	Bottoms	24	165	1.00	l	1.21E+04	3.36	0	0	280	0	0	1.18E+04	0	0	0	0	0	0	3.04
		28	165	6.00	l	3358	3358	0	0	0	0	0	0	0	0	0	0	0	0	0
Display in PFD	Feed	24	165	1.00	l	1.21E+04	3.36	0	0	280	0	0	1.18E+04	0	0	0	0	0	0	3.04
Di <4>		percentage of input in distillate			:		100			3.00			99.9							100

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Cumene	Cumene Hydroperoxide	DMBA	acetophenone	alpha-methylstyrene	Dicumyl Peroxide	Phenol	Acetone	Air	Nitrogen	Oxygen	Hydrogen	Methanol	Water
		percentage of input in bottoms			:		0	100	100	97.0	100	100	0.1000	100	100	100	100	100	100	0
		Boiling Temperature (Tb) [oC]	182		:		152			203			182							100
Distillate		25	182	1.00	l	1.18E+04	3.36	0	0	8.39	0	0	1.18E+04	0	0	0	0	0	0	3.04
Display in PFD	Bottoms	26	182	1.00	l	283	0	0	0	271	0	0	11.8	0	0	0	0	0	0	0
Feed		26a	25.0	1.00	l	283	0	0	0	271	0	0	11.8	0	0	0	0	0	0	0
Di <5>		percentage of input in distillate			:					88.5			0							
		percentage of input in bottoms			:		100	100	100	11.5	100	100	100	100	100	100	100	100	100	100
		Boiling Temperature (Tb) [oC]			:					202			182							
Distillate		26b	134	0.132	l	240	0	0	0	240	0	0	0	0	0	0	0	0	0	0
Bottoms		26e	134	0.132	l	43.1	0	0	0	31.2	0	0	11.8	0	0	0	0	0	0	0
		26c	134	1.00	l	240	0	0	0	240	0	0	0	0	0	0	0	0	0	0
By-product		26d	25.0	1.00	l	-240	0	0	0	-240	0	0	0	0	0	0	0	0	0	0
		26f	134	1.00	l	43.1	0	0	0	31.2	0	0	11.8	0	0	0	0	0	0	0
Waste		26g	25.0	1.00	l	-43.1	0	0	0	-31.2	0	0	-11.8	0	0	0	0	0	0	0
By-product	0.999	27	25.0	1.00	l	-1.18E+04	-3.36	0	0	-8.39	0	0	-1.18E+04	0	0	0	0	0	0	-3.04
		Product purity (%)			:	0.997														
		Main product			:	alpha-methylstyrene														
		Overall Rxn coefficients			:		-1.00				1.00						-0.500			1.00
		Total yield of process (from reactant)			:		6.11				NA						NA			NA
Waste		Fug. loss			g	-156	0	0	0	0	0	0	0	-148	0	0	0	0	-8.50	0
		Input Sum			:	3.50E+04	1.66E+04	0	0	0	0	0	0	0	1.84E+04	0	0	0	0	0
		Replacement of fugitive emissions of reactants			:	0	0										0			
		Total Input (Input + Fugitive Replacement)			:	3.50E+04	1.66E+04	0	0	0	0	0	0	0	1.84E+04	0	0	0	0	0
		Product Sum			:	2.06E+04	23.6	0	0	249	998	0	1.20E+04	7384	0	0	0	0	7.39E-03	32.9
		Main product flow			:	1000	3.36	0	0	0	997	0	0	0	0	0	0	0	0	0
		Net Input (in - out, omitting fugitives)			:	-7.16E-03														

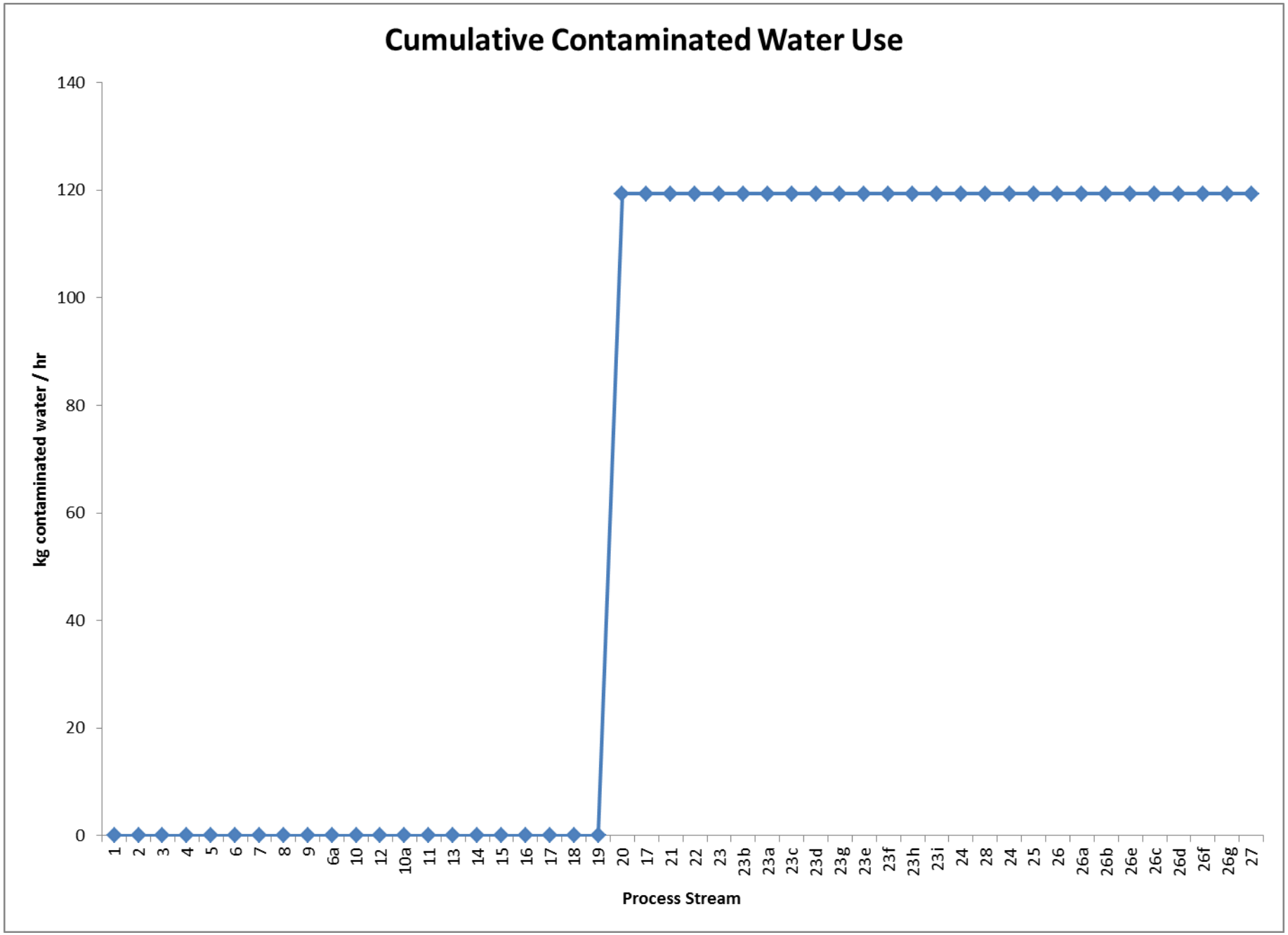
Type	Label	Temp, C	P, atm	Phase	Total flow	Steam	Water
Input	C1	20.0	1.00	l	1.03E+04		1.03E+04
Cooling out	C2	50.0	1.00	l	-1.03E+04		-1.03E+04
Input	C3	20.0	1.00	l	1.25E+05		1.25E+05
Cooling out	C4	50.0	1.00	l	-1.25E+05		-1.25E+05
Input	C5	20.0	1.00	l	1.80E+05		1.80E+05
Cooling out	C6	50.0	1.00	l	-1.80E+05		-1.80E+05
Input	C7	20.0	1.00	l	6978		6978
Cooling out	C8	50.0	1.00	l	-6978		-6978
Input	C9	20.0	1.00	l	1.91E+05		1.91E+05
Cooling out	C10	50.0	1.00	l	-1.91E+05		-1.91E+05
Input	C11	20.0	1.00	l	2.77E+04		2.77E+04
Cooling out	C12	50.0	1.00	l	-2.77E+04		-2.77E+04

Input	C13	20.0	1.00	l	8577		8577
Cooling out	C14	50.0	1.00	l	-8577		-8577
Input	C15	20.0	1.00	l	6.74E+04		6.74E+04
Cooling out	C16	50.0	1.00	l	-6.74E+04		-6.74E+04
Input	C17	20.0	1.00	l	1.07E+05		1.07E+05
Cooling out	C18	50.0	1.00	l	-1.07E+05		-1.07E+05
Input	C19	20.0	1.00	l	2.80E+04		2.80E+04
Cooling out	C20	50.0	1.00	l	-2.80E+04		-2.80E+04
Input	C21	20.0	1.00	l	1.33E+04		1.33E+04
Cooling out	C22	50.0	1.00	l	-1.33E+04		-1.33E+04
Input	C23	50.0	1.00	l	821		821
Cooling out	C24	50.0	1.00	l	-821		-821
Input	C25	50.0	1.00	l	3.62E+04		3.62E+04
Cooling out	C26	50.0	1.00	l	-3.62E+04		-3.62E+04
Input	C27	50.0	1.00	l	6928		6928
Cooling out	C28	50.0	1.00	l	-6928		-6928
Input	C29	50.0	1.00	l	1625		1625
Cooling out	C30	50.0	1.00	l	-1625		-1625
Input	S1	207	1.00	l	1.64E+04	1.64E+04	
Steam out	S2	207	1.00	l	-1.64E+04	-1.64E+04	
Input	S3	207	1.00	l	3054	3054	
Steam out	S4	207	1.00	l	-3054	-3054	
Input	S5	207	1.00	l	7494	7494	
Steam out	S6	207	1.00	l	-7494	-7494	
Input	S7	207	1.00	l	1.00E+04	1.00E+04	
Steam out	S8	207	1.00	l	-1.00E+04	-1.00E+04	
Input	S9	207	1.00	l	1242	1242	
Steam out	S10	207	1.00	l	-1242	-1242	
Input	S11	207	1.00	l	3295	3295	
Steam out	S12	207	1.00	l	-3295	-3295	
Input	S13	207	1.00	l	644	644	
Steam out	S14	207	1.00	l	-644	-644	

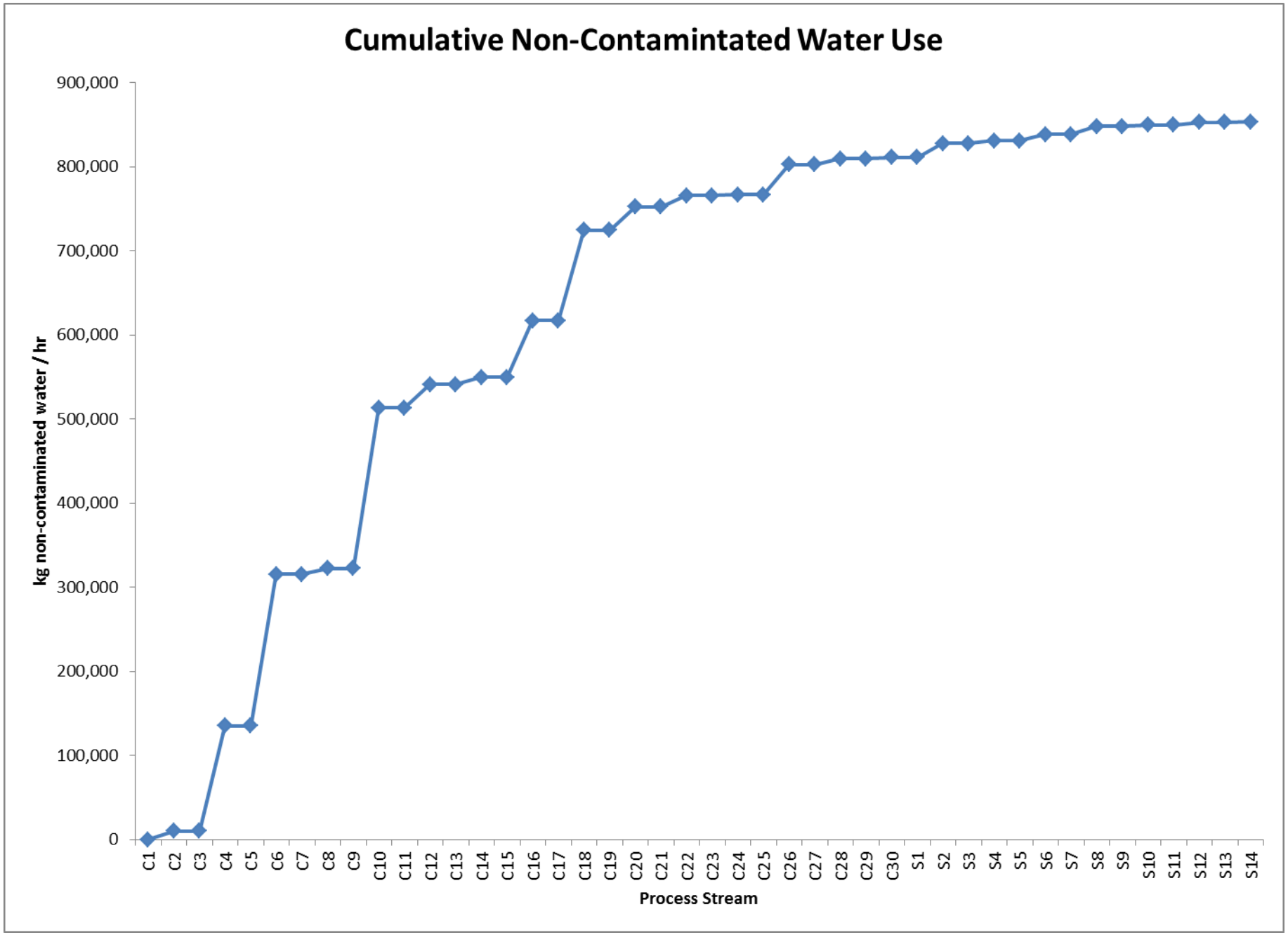
Graph of Cumulative Chemical Losses through Manufacturing Process



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	17.5	17.5		E	R1	Reactor 1	-1.84E+04	-1.84E+04	100	0.250	-4612	-4612
Cmp1	Compressor 1	4913	4930		E	Hx1	Heat exchanger 1	-1524	-2.00E+04	100	0.250	-381	-4993
P2	Pump 2	79.4	5010		E	Di1	Distillation condenser 1	-2.66E+04	-4.66E+04	100	0.250	-6658	-1.17E+04
P3	Pump 3	5.96	5015		E	Hx2	Heat exchanger 2	-1030	-4.76E+04	100	0.250	-258	-1.19E+04
Vac1	Vacuum electricity 1	19.3	5035		E	R2	Reactor 2	-2.82E+04	-7.58E+04	80.0	0.250	-7053	-1.90E+04
P4	Pump 4	3.36	5038		E	Di2	Distillation condenser 2	-4084	-7.99E+04	98.9	0.250	-1021	-2.00E+04
Di1	Distillation reboiler 1	2.66E+04	3.17E+04	100	S	Hx3	Heat exchanger 3	-1267	-8.12E+04	100	0.250	-317	-2.03E+04
Di2	Distillation reboiler 2	4964	3.66E+04	98.9	S	Di3	Distillation condenser 3	-9948	-9.11E+04	164	0.450	-4476	-2.48E+04
Di3	Distillation reboiler 3	1.22E+04	4.88E+04	164	S	Hx3a	Heat exchanger 3a	-121	-9.13E+04	165	0.450	-54.5	-2.48E+04
Di3a	Distillation reboiler 3a	5356	5.42E+04	151	S	Di3a	Distillation condenser 3a	-5349	-9.66E+04	151	0.450	-2407	-2.72E+04
P4a	Pump 4a	0.0109	5.42E+04		E	Di3b	Distillation condenser 3b	-1023	-9.76E+04	164	0.450	-460	-2.77E+04
P4b	Pump 4b	6.71E-04	5.42E+04		E	Hx3b	Heat exchanger 3b	-240	-9.79E+04	165	0.450	-108	-2.78E+04
Di3b	Distillation reboiler 3b	1046	5.52E+04	164	S	Di4	Distillation condenser 4	-1.58E+04	-1.14E+05	181	0.450	-7128	-3.49E+04
P4c	Pump 4c	0.0723	5.52E+04		E	Hx4	Heat exchanger 4	-4133	-1.18E+05	182	0.450	-1860	-3.68E+04
P4d	Pump 4d	9.37E-07	5.52E+04		E	Di5	Distillation condenser 5	-1960	-1.20E+05	134	0.250	-490	-3.73E+04
Di4	Distillation reboiler 4	1.63E+04	7.15E+04	181	S								
P5	Pump 5	9.86E-06	7.15E+04		E								
Vac2	Vacuum electricity 2	23.7	7.15E+04		E								
Di5	Distillation reboiler 5	2019	7.35E+04	134	S								
P6	Pump 6	0.0349	7.35E+04		E								
P7	Pump 7	6.26E-03	7.35E+04		E								
	Potential recovery	-3.73E+04	3.62E+04										
	Net energy		3.62E+04				Potential recovery:						-3.73E+04

Electricity	5062	E	[MJ/hr]
Heating steam	6.85E+04	S	[MJ/hr]
Energy input requirement	7.35E+04		[MJ/hr]
Cooling water	-1.20E+05		[MJ/hr]
Potential heat recovery	-3.73E+04		[MJ/hr]
Net energy	3.62E+04		[MJ/hr]

Graph of Cumulative Energy Requirements