Acrolein from propylene and oxygen from air [107-02-8]

CONTENTS OF FACTORY GATE TO FACTORY GATE

LIFE CYCLE INVENTORY SUMMARY

Authors	Y. Li
Peer reviews, name (date)	Reviewed by MR Overcash on 9-7-2007: route, stoichiometry, and calculations reviewed and found to be representative. Reviewed by EM Griffing on 9-1-2016: route and stoichiometry reviewed and found to be representative.
Gtg report last modified on	9-1-2016
Additional notes	

Checked for database consistency on	9-1-2016
First gtg version finalized on	9-7-2007
Modification history, Author (date)	EMG (9-1-2016) and YL (9-7-2007)

Products	Acrolein, Acrylic acid, Acetic acid
Standard inputs	oxygen from air, Propylene

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.

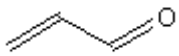
Chemistry

Primary reaction:

$CH_2CHCH_3 + O_2 \rightarrow CH_2CHCHO + H_2O$ (1-1)

Propylene

Oxygen



Acrolein

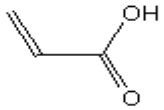
Water

Side reactions:

$CH_2CHCH_3 + 1.5O_2 \rightarrow CH_2CHCOOH + H_2O$ (1-2)

Propylene

Oxygen



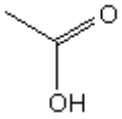
Acrylic acid

Water

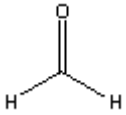
$CH_2CHCH_3 + 1.5O_2 \rightarrow CH_3COOH + CH_2O$ (1-3)

Propylene

Oxygen



Acetic acid

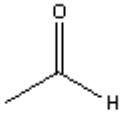


Formaldehyde

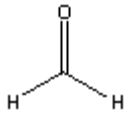
$CH_2CHCH_3 + O_2 \rightarrow C2H4O + CH_2O$ (1-4)

Propylene

Oxygen



Acetaldehyde



Formaldehyde

Griffing and Overcash, Chemical Life Cycle Database, www.environmentalclarity.com, 1999-present.

Process Summary

Literature

"Acrolein is a colorless, volatile, toxic, and lacrimatory liquid with a powerful odor. The commercial production of acrolein by heterogeneously catalyzed gas-phase condensation of acetaldehyde and formaldehyde was established by Degussa in 1942. Today, acrolein is produced on a large commercial scale by heterogeneously catalyzed gas-phase oxidation of propene."[1]

LCI design

Propylene, air, and steam are compressed to 2 atm and then mixed at a molar ratio of 1:8:4[2]. The gas mixture is fed to a multitubular fixed-bed reactor, which is operated at 350 ^{o}C and 2 atm[2]. The conversion rate of propylene in this reactor is 95%[2].

The effluent gas from the reactor is cooled to 250 ^{o}C and then fed into a gas washer. An aqueous stream and an organic liquid, 2-ethylhexanol, are used to wash the gas stream. The ratio of gas stream:aqueous stream:organic stream is 10.6:1.5:1[3]. The residual gas leaves gas washer at 70 ^{o}C and is introduced to the bottom of a gas cooler. The liquid stream from the gas washer is pumped into series of distillation columns at 105 ^{o}C to recover byproducts acrylic acid and acetic acid [3]. From the gas cooler, the residual gas stream leaves at 19 ^{o}C and is fed into another gas washer to recover residual acrolein. The organic phase from the bottom of the cooler is recycled to the first gas washer at 45 ^{o}C[3]. Part of the aqueous phase is combined with the organic phase of the second gas washer and cooled to 16 ^{o}C and recycled to the gas cooler. Part of the aqueous phase from the gas cooler is recycled to the first gas washer. The second gas washer using water-2-ethylhexanol mixture to wash the residual gas at 2^{o}C[3]. The aqueous phase is then combined with part of the aqueous phase from the gas cooler to recover acrolein product. 2-Ethylhexanol is also recovered and combined with makeup 2-ethylhexanol and water. This stream is cooled to 2 ^{o}C and fed into the second gas washer.

Route review 2016

KO (2009), KO (2007), and KO (2015) confirm propylene oxide as only commercial route.

Critical parameters

Conversion / Yield information from both reactors			
		Conversion of or Yield from Propylene	Conversion of or Yield from Oxygen
Total conversion in reactor 1: (% of reactant entering the process that reacts)	From mass balance	95	60
Total per pass conversion in reactor 1:	From mass	95	60

[1] Acrolein and Methacrolein, Ullmann's Encyclopedia of Industrial Chemistry, online edition, pp 1
[2] Acrolein and Methacrolein, Ullmann's Encyclopedia of Industrial Chemistry, online edition, pp 6-7
[3] US patent 3,926,744, Dec. 16, 1975

(% of reactant entering the reactor that reacts)	balance		
Total yield of reactor 1: (% yield acrolein produced in the reactor based on reactant input to process)	From mass balance	86	81
Total yield of Process: (% yield produced by the overall process based on reactant input to process)	From mass balance	76	46
Notes:			

Product purity			
	Acrolein		Comments
Used here	98.6%		
LiteratureSource			

Summary of LCI Information

Inputs

UID	CAS	Chemical	Amount	Purity (%)	Units	Comments
UIDO2FromAir	7782-44-7	Oxygen from air	736	100	[kg/hr]	
115-07-1	Propylene	Propylene	979	100	[kg/hr]	
		Total	1,715		[kg/hr]	

Non-reacting inputs

UID	CAS	Chemical	Amount	Purity (%)	Units	Comments
UIDN2FromAir	7727-37-9	Nitrogen from air	4039		[kg/hr]	
7732-18-5	7732-18-5	Water	9,644		[kg/hr]	
UIDO2FromAir	7782-44-7	Oxygen from air	491		[kg/hr]	
		Total non-reacting inputs	14,174		[kg/hr]	

Ancillary inputs

UID	CAS	Chemical	Amount	Purity (%)	Units	Comments
104-76-7	104-76-7	Ethylhexanol, 2	9	100	[kg/hr]	
		Total ancillary inputs	9		[kg/hr]	

Products

UID	CAS	Chemical	Amount	Purity (%)	Units	Comments
107-02-8	107-02-8	Acrolein	1,000	99.5	[kg/hr]	
79-10-7	79-10-7	Acrylic acid	145	96.4	[kg/hr]	
64-19-7	64-19-8	Acetic acid	51	65.4	[kg/hr]	
		Total	1196		[kg/hr]	

Benign outflows

UID	CAS	Chemical	Amount	Purity (%)	Units	Comments
7727-37-9	7727-37-9	Nitrogen	4,039		[kg/hr]	
7782-44-7	7782-44-7	Oxygen	491		[kg/hr]	
7732-18-5	7732-18-5	Water	10,036		[kg/hr]	
		Total benign output flows	14565		[kg/hr]	

Chemical Emissions

UID	CAS	Chemical	Amount				Units	Comments
			Gas	Liquid	Solid	Solvent		
79-10-7	79-10-7	Acrylic acid		0.740			[kg/hr]	
107-02-8	107-02-8	Acrolein	19.9	56.0			[kg/hr]	
115-07-1	115-07-1	Propylene	66.7	0.480			[kg/hr]	
64-19-7	64-19-7	Acetic acid	0.343	0.343			[kg/hr]	
50-00-0	50-00-0	Formaldehyde	27.5	0.0274			[kg/hr]	
75-07-0	75-07-0	Acetaldehyde	15.0	0.0151			[kg/hr]	
104-76-7	104-76-7	Ethylhexanol, 2		5.56			[kg/hr]	
		Total	129.4	63.1	0	0	[kg/hr]	
	Mass Balance Difference		-57				[kg/hr]	

Energy use

Source	Amount	Units	Comments
Electricity	2045	[MJ/hr]	
Dowtherm	0	[MJ/hr]	
Heating steam	2.10E+04	[MJ/hr]	85% efficiency has been included to determine how much steam is needed for heating process fluid
Direct fuel use in high temperature heating	0	[MJ/hr]	
Heating natural gas	0	[MJ/hr]	
Energy input requirement	2.31E+04	[MJ/hr]	Electricity + steam + direct fuel oil + Dowtherm
Cooling water	-1.92E+04	[MJ/hr]	
Cooling refrigeration	0	[MJ/hr]	
Potential Heat Recovery	-4417	[MJ/hr]	
Net energy	1.86E+04	[MJ/hr]	Energy input requirement minus potential heat recovery from cooling systems.

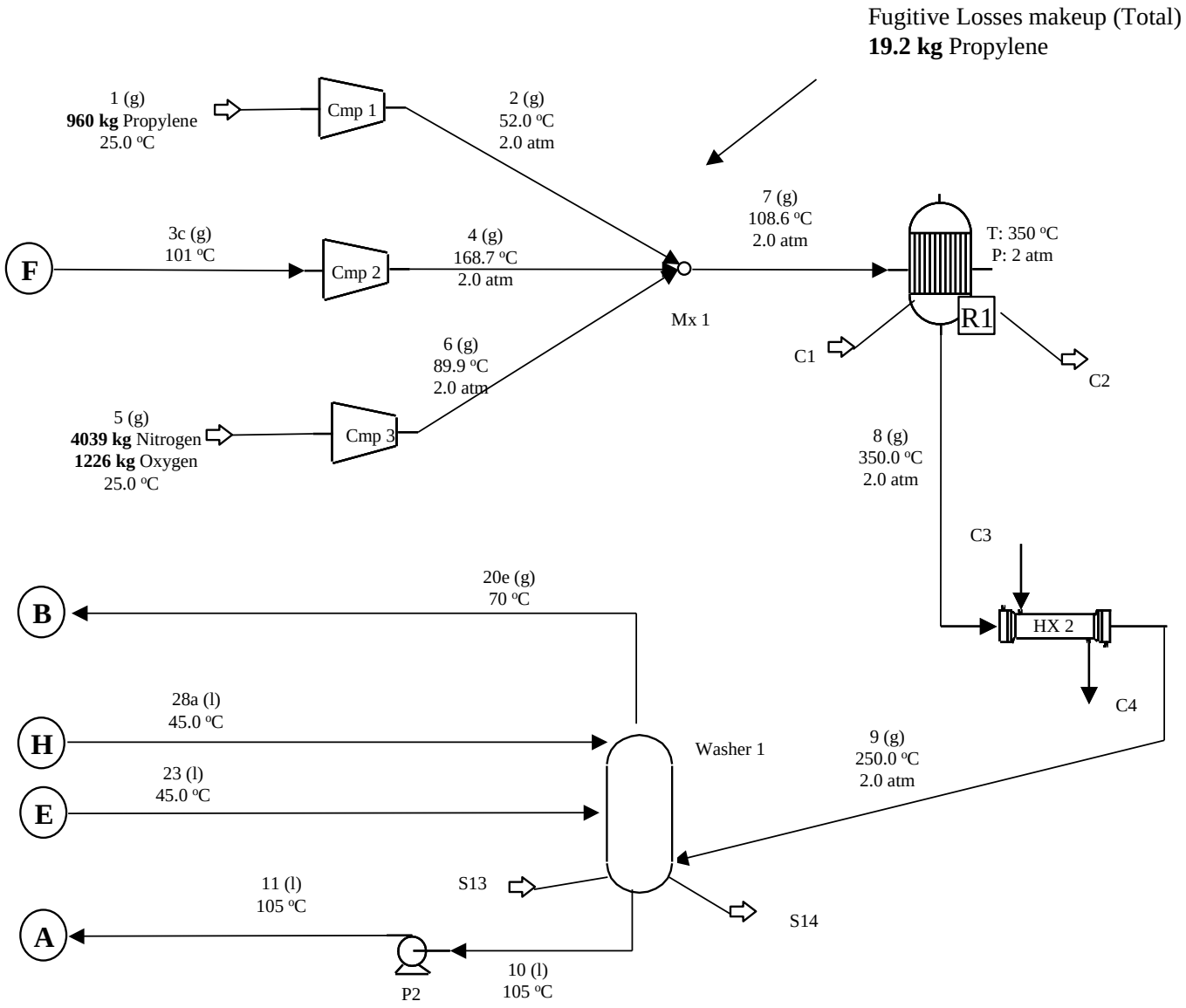
Process Diagram Interpretation Sheet

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

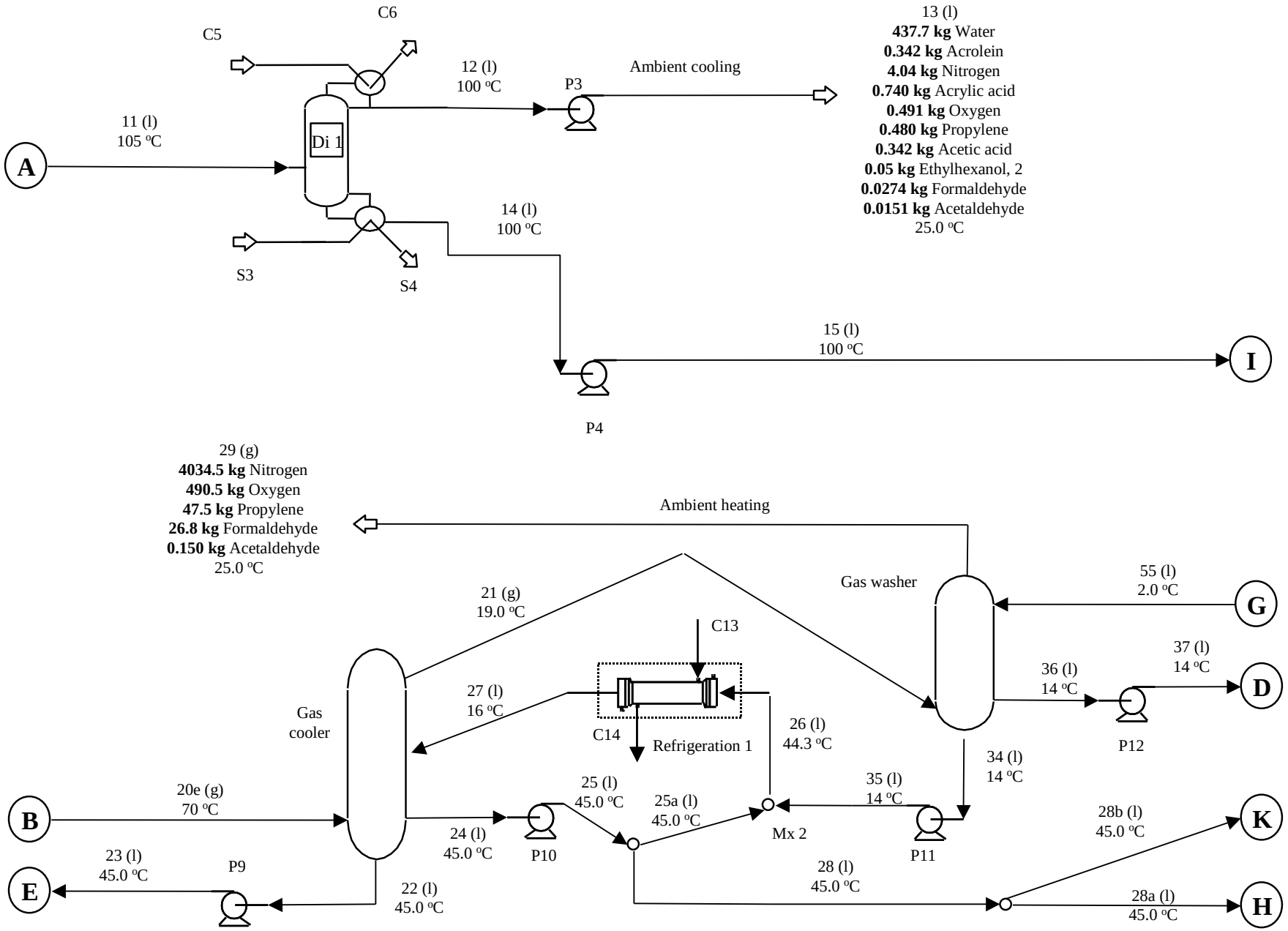
For most streams, the temperature and pressure are shown, if the pressures are greater than 1 atm

Process Diagram or Boundary of LCI

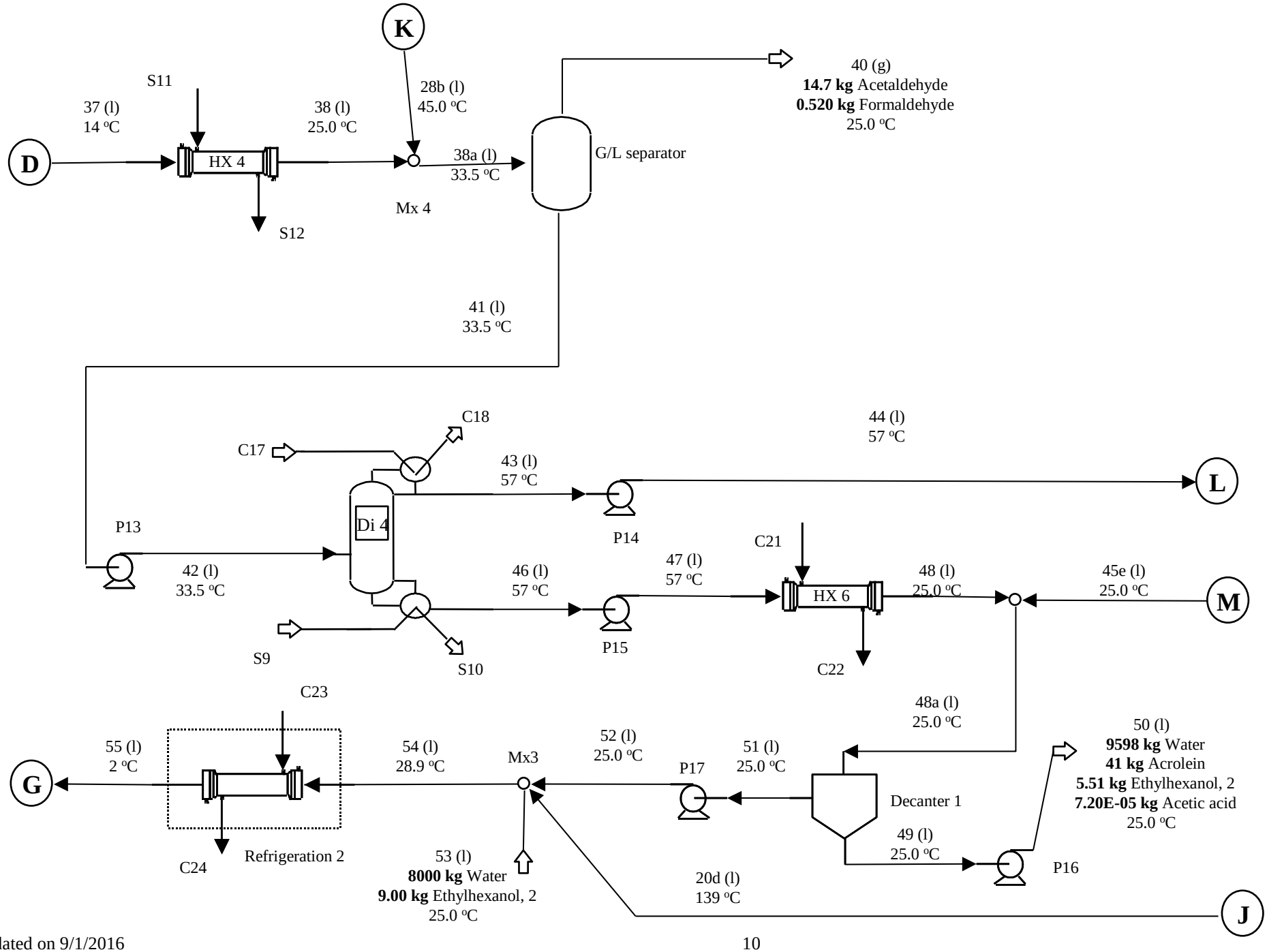
Steam enters the process as a gas at 207 °C and leaves as a liquid at 207 °C. Cooling water enters at 20 °C and leaves at 50 °C.
Unless otherwise indicated, all processes are at 1 atm.

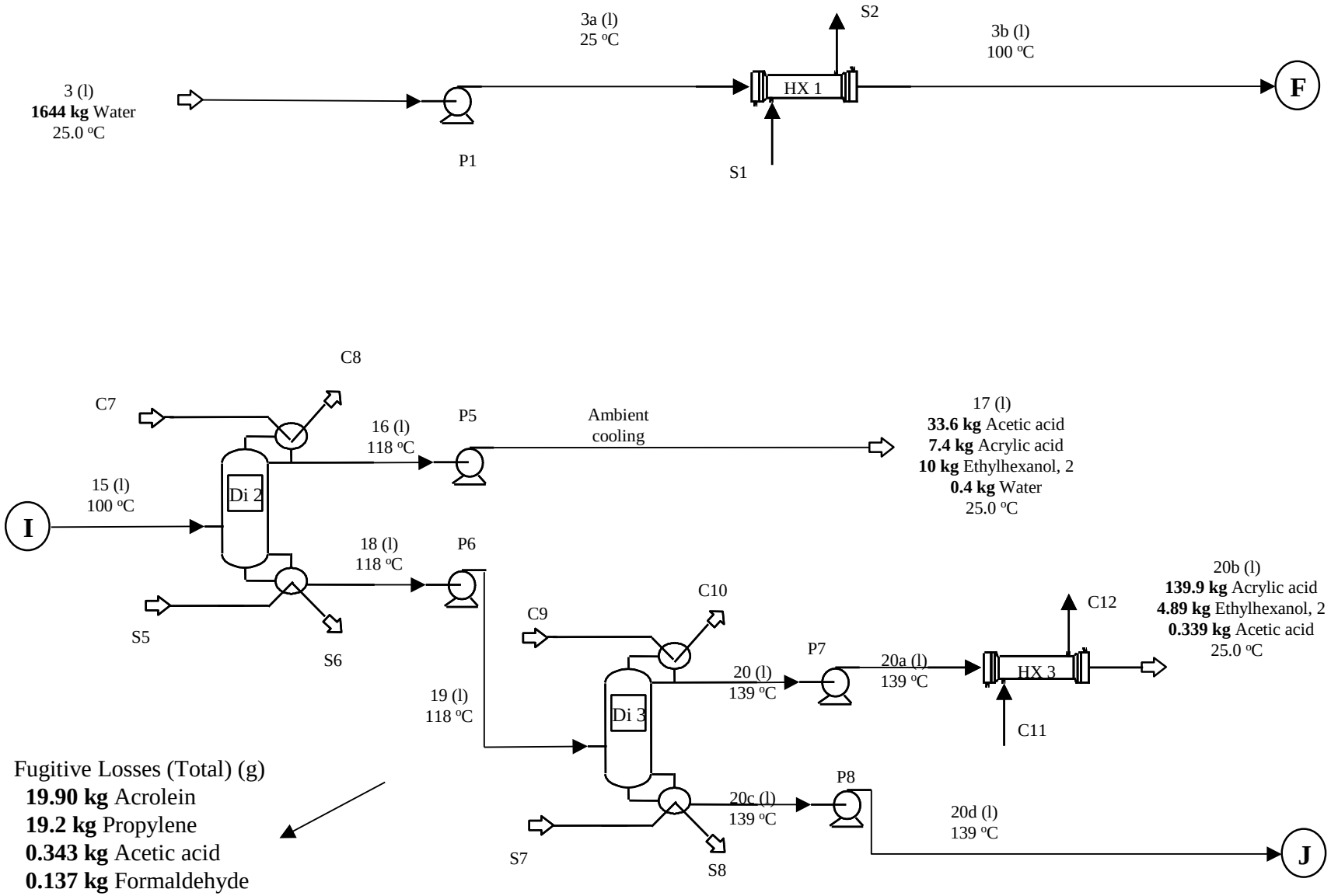


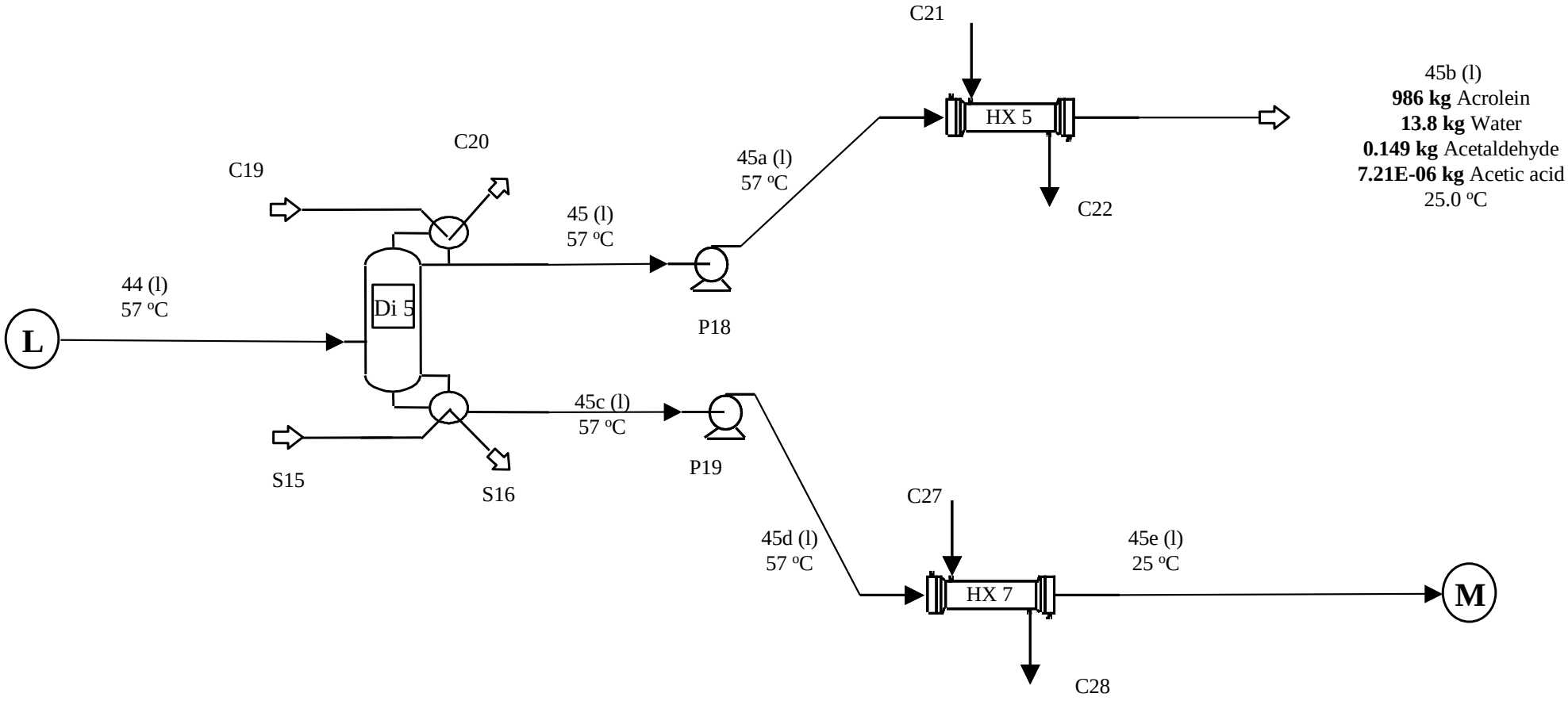
Griffing and Overcash, Chemical Life Cycle Database, www.environmentalclarity.com, 1999-present.



Griffing and Overcash, Chemical Life Cycle Database, www.environmentalclarity.com, 1999-present.


K
S11
37 (l)
14 ºC
28b (l)
45.0 ºC
38 (l)
25.0 ºC
40 (g)
14.7 kg Acetaldehyde
0.520 kg Formaldehyde
25.0 ºC
D
HX 4
38a (l)
33.5 ºC
G/L separator
Mx 4
S12
41 (l)
33.5 ºC
C18
44 (l)
57 ºC
C17
43 (l)
57 ºC
L
P13
Di 4
P14
C21
42 (l)
33.5 ºC
46 (l)
57 ºC
47 (l)
57 ºC
HX 6
48 (l)
25.0 ºC
45e (l)
25.0 ºC
M
S9
S10
P15
C22
C23
48a (l)
25.0 ºC
50 (l)
9598 kg Water
41 kg Acrolein
5.51 kg Ethylhexanol, 2
7.20E-05 kg Acetic acid
25.0 ºC
55 (l)
2 ºC
54 (l)
28.9 ºC
Mx3
52 (l)
25.0 ºC
P17
51 (l)
25.0 ºC
G
Decanter 1
49 (l)
25.0 ºC
P16
C24
Refrigeration 2
53 (l)
8000 kg Water
9.00 kg Ethylhexanol, 2
25.0 ºC
20d (l)
139 ºC
J


3 (l)
1644 kg Water
25.0 ºC
P1
3a (l)
25 ºC
S2
HX 1
S1
3b (l)
100 ºC
F
C8
C7
16 (l)
118 ºC
P5
Ambient
cooling
17 (l)
33.6 kg Acetic acid
7.4 kg Acrylic acid
10 kg Ethylhexanol, 2
0.4 kg Water
25.0 ºC
15 (l)
100 ºC
I
Di 2
18 (l)
118 ºC
P6
S5
S6
C9
C10
C12
20b (l)
139.9 kg Acrylic acid
4.89 kg Ethylhexanol, 2
0.339 kg Acetic acid
25.0 ºC
P7
20 (l)
139 ºC
20a (l)
139 ºC
HX 3
C11
19 (l)
118 ºC
Di 3
P8
20c (l)
139 ºC
20d (l)
139 ºC
S7
S8
J
Fugitive Losses (Total) (g)
19.90 kg Acrolein
19.2 kg Propylene
0.343 kg Acetic acid
0.137 kg Formaldehyde
0.0753 kg Acetaldehyde



Griffing and Overcash, Chemical Life Cycle Database, www.environmentalclarity.com, 1999-present.

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, atm	Phase	Total Flow	Acrylic acid	Oxygen	Acrolein	Propylene	Water	Acetic acid	Formaldehyde	Nitrogen	Acetaldehyde	Ethylhexanol, 2	Steam	Water
Input		1	25.0	1.00	g	960				960								
		2	52.0	2.00	g	960				960								
Input		3	25.0	1.00	l	1644					1644							
		3a	25.0	1.00	l	1644					1644							
		3b	100	1.00	g	1644					1644							
		4	169	2.00	g	1644					1644							
Input		5	25.0	1.00	g	5265		1226						4039				
		6	89.9	2.00	g	5265		1226						4039				
		7	109	2.00	g	7869		1226	0	960	1644	0	0	4039	0	0		
R1	787	kg	Propylene			is converted in rxn 1 (82.0 % of reactor input)												
	86.4	kg	Propylene			is lost in rxn 2												
	24.0	kg	Propylene			is lost in rxn 3												
	14.4		Propylene			is lost in rxn 4												
		Input to reactor			:	7869	0	1226	0	960	1644	0	0	4039	0	0		
		R1 Reaction Coefficient 1			:			-1.00	1.00	-1.00	1.00							
		R1 Conversion 1 [kg/hr]			:	-0.374		-599	1049	-787	337							
		R1 Conversion 1 [kgmol/hr]			:	18.7		-18.7	18.7	-18.7	18.7							
		R1 Reaction Coefficient 2			:		1.00	-1.50		-1.00	1.00							
		R1 Conversion 2 [kg/hr]			:	-0.0341	148	-98.6		-86.4	37.0							
		R1 Conversion 2 [kgmol/hr]			:	2.05	2.05	-3.08		-2.05	2.05							
		R1 Reaction Coefficient 3			:			-1.50		-1.00		1.00	1.00					
		R1 Conversion 3 [kg/hr]			:	1.37E-03		-27.4		-24.0		34.3	17.1					
		R1 Conversion 3 [kgmol/hr]			:	0.570		-0.856		-0.570		0.570	0.570					

	Comments	Streams	Temp [C]	P, atm	Phase	Total Flow	Acrylic acid	Oxygen	Acrolein	Propylene	Water	Acetic acid	Formaldehyde	Nitrogen	Acetaldehyde	Ethylhexanol, 2	Steam	Water
		R1 Reaction Coefficient 4			:			-1.00		-1.00			1.00		1.00			
		R1 Conversion 4 [kg/hr]			:	-0.0171		-11.0		-14.4			10.3		15.1			
		R1 Conversion 4 [kgmol/hr]			:	0.342		-0.342		-0.342			0.342		0.342			
		Flow out of reactor			:	7869	148	491	1049	48.0	2018	34.3	27.4	4039	15.1	0		
		Primary product			:	Acrolein												
		Total conversion			:		NA	60.0	NA	95.0		NA	NA	-0	NA	-0		
		Per pass conversion			:		NA	60.0	NA	95.0	NA	NA	NA	-0	NA			
		Total yield from reactor			:			81.4	NA	86.3								
		8	350	2.00	g	7869	148	491	1049	48.0	2018	34.3	27.4	4039	15.1	0		
		9	250	2.00	g	7869	148	491	1049	48.0	2018	34.3	27.4	4039	15.1	0		
		Stream 28a:Recycle input				1104			320		784					0.100		
		Stream 28a:Recycle calculated				1098	0	0	319	0	780	0	0	0	0	0.134		
		Stream 28a:Recycle residue				5.87	0	0	1.43	0	4.47	0	0	0	0	-0.0341		
		Stream 23:Recycle input				743			122		119	1.80				500		
		Stream 23:Recycle calculated				743	0	0	124	0	118	1.78	0	0	0	500		
		Stream 23:Recycle residue				-0.943	0	0	-1.68	0	0.769	0.0155	0	0	0	-0.0491		
		10	105	1.00	l	1140	148	0.491	14.9	0.480	438	34.2	0.0274	4.04	0.0151	500		
		11	105	1.00	l	1140	148	0.491	14.9	0.480	438	34.2	0.0274	4.04	0.0151	500		
	Feed	11	105	1.00	l	1140	148	0.491	14.9	0.480	438	34.2	0.0274	4.04	0.0151	500		
		streamphase					l	g	g	g	g	l	g	g	g	l		
Di <1>		percentage of input in distillate			:		0.500	100	100	100	99.9	1.00	100	100	100	0.0100		
		percentage of input in bottoms			:		99.5	0	0	0	0.1000	99.0	0	0	0	100.0		
		Boiling Temperature (Tb) [oC]			:		139	-183	56.9	-47.7	99.9	118	-19.2	-194	20.9	183		
	Distillate	12	100	1.00	l	459	0.740	0.491	14.9	0.480	438	0.342	0.0274	4.04	0.0151	0.0500		
		streamphase					l	g	g	g	l	l	g	g	g	l		
	Bottoms	14	100	1.00	l	681	147	0	0	0	0.438	33.9	0	0	0	500		
		streamphase					l	g	g	g	l	l	g	g	g	l		
		12	100	1.00	l	459	0.740	0.491	14.9	0.480	438	0.342	0.0274	4.04	0.0151	0.0500		
Waste		13	25.0	1.00	l	-459	-0.740	-0.491	-14.9	-0.480	-438	-0.342	-0.0274	-4.04	-0.0151	-0.0500	0	0

	Comments	Streams	Temp [C]	P, atm	Phase	Total Flow	Acrylic acid	Oxygen	Acrolein	Propylene	Water	Acetic acid	Formaldehyde	Nitrogen	Acetaldehyde	Ethylhexanol, 2	Steam	Water
		14	100	1.00	l	681	147	0	0	0	0.438	33.9	0	0	0	500		
		15	100	1.00	l	681	147	0	0	0	0.438	33.9	0	0	0	500		
	Feed	15	100	1.00	l	681	147	0	0	0	0.438	33.9	0	0	0	500		
		streamphase					l	g	g	g	l	l	g	g	g	l		
Di <2>		percentage of input in distillate			:		5.00	100	100	100	100	99.0	100	100	100	2.00		
		percentage of input in bottoms			:		95.0	0	0	0	0	1.00	0	0	0	98.0		
		Boiling Temperature (Tb) [oC]			:		139	-183	56.9	-47.7	99.9	118	-19.2	-194	20.9	183		
	Distillate	16	118	1.00	l	51.4	7.36	0	0	0	0.438	33.6	0	0	0	9.99		
		streamphase					l	g	g	g	l	l	g	g	g	l		
	Bottoms	17a	118	1.00	l	630	140	0	0	0	0	0.339	0	0	0	490		
		streamphase					l	g	g	g	l	l	g	g	g	l		
		16	118	1.00	l	51.4	7.36	0	0	0	0.438	33.6	0	0	0	9.99		
By-product		17	25.0	1.00	l	-51.4	-7.36	0	0	0	-0.438	-33.6	0	0	0	-9.99	0	0
		18	118	1.00	l	630	140	0	0	0	0	0.339	0	0	0	490		
		19	118	1.00	l	630	140	0	0	0	0	0.339	0	0	0	490		
	Feed	19	118	1.00	l	630	140	0	0	0	0	0.339	0	0	0	490		
		streamphase					l	g	g	g	g	l	g	g	g	l		
Di <3>		percentage of input in distillate			:		100	100	100	100	100	100	100	100	100	1.00		
		percentage of input in bottoms			:		0	0	0	0	0	0	0	0	0	99.0		
		Boiling Temperature (Tb) [oC]			:		139	-183	56.9	-47.7	99.9	118	-19.2	-194	20.9	183		
	Distillate	20	139	1.00	l	145	140	0	0	0	0	0.339	0	0	0	4.90		
		streamphase					l	g	g	g	g	g	g	g	g	l		
	Bottoms	20c	139	1.00	l	485	0	0	0	0	0	0	0	0	0	485		
		streamphase					l	g	g	g	g	g	g	g	g	l		
		20	139	1.00	l	145	140	0	0	0	0	0.339	0	0	0	4.90		
		20a	139	1.00	l	145	140	0	0	0	0	0.339	0	0	0	4.90		
By-product		20b	25.0	1.00	l	-145	-140	0	0	0	0	-0.339	0	0	0	-4.90	0	0
		20d	139	1.00	l	485	0	0	0	0	0	0	0	0	0	485		
		20e	70.0	1.00	g	8576	0	490	1476	47.5	2483	1.80	27.4	4035	15.0	0.500		
		Stream 27:Recycle input				3.84E+04			1.09E+04		2.70E+04					505		
		Stream 27:Recycle				3.84E+04	0	0	1.09E+04	0	2.70E+04	0	0	0	0	505		

	Comments	Streams	Temp [C]	P, atm	Phase	Total Flow	Acrylic acid	Oxygen	Acrolein	Propylene	Water	Acetic acid	Formaldehyde	Nitrogen	Acetaldehyde	Ethylhexanol, 2	Steam	Water
		calculated																
		Stream 27:Recycle residue				-16.7	0	0	-4.11	0	-12.5	0	0	0	0	-0.0263		
		21	19.0	1.00	g	4871	0	490	247	47.5	8.84	0.0180	27.4	4035	15.0	0		
		22	45.0	1.00	l	743	0	0	124	0	118	1.78	0	0	0	500		
		23	45.0	1.00	l	743	0	0	124	0	118	1.78	0	0	0	500		
		24	45.0	1.00	l	4.14E+04	0	0	1.20E+04	0	2.94E+04	0	0	0	0	5.05		
		25	45.0	1.00	l	4.14E+04	0	0	1.20E+04	0	2.94E+04	0	0	0	0	5.05		
		25a	45.0	1.00	l	3.74E+04	0	0	1.09E+04	0	2.66E+04	0	0	0	0	4.57		
		Stream 35:Recycle input				931			24.8		406					500		
		Stream 35:Recycle calculated				924	0	0	24.8	0	406	0.0108	0.0274	0	0	493		
		Stream 35:Recycle residue				-6.93	0	0	-0.0144	0	-0.158	0.0108	0.0274	0	0	-6.80		
		26	44.3	1.00	l	3.84E+04	0	0	1.09E+04	0	2.70E+04	0	0	0	0	505		
		27	16.0	1.00	l	3.84E+04	0	0	1.09E+04	0	2.70E+04	0	0	0	0	505		
		28	45.0	1.00	l	3908	0	0	1134	0	2774	0	0	0	0	0.477		
		28a	45.0	1.00	l	1098	0	0	319	0	780	0	0	0	0	0.134		
		28b	45.0	1.00	l	2810	0	0	815	0	1995	0	0	0	0	0.343		
		Stream 55:Recycle input				8651			0.500		8102					548		
		Stream 55:Recycle calculated				8642	0	0	2.16	0	8097	7.14E-03	0	0	0	543		
		Stream 55:Recycle residue				8.09	0	0	-1.66	0	5.05	-7.14E-03	0	0	0	4.71		
Waste		29	25.0	1.00	g	-4599	0	-490	0	-47.5	0	0	-26.8	-4035	-0.150	0	0	0
		34	14.0	1.00	l	924	0	0	24.8	0	406	0.0108	0.0274	0	0	493		
		35	14.0	1.00	l	924	0	0	24.8	0	406	0.0108	0.0274	0	0	493		
		36	14.0	1.00	l	7999	0	0	223	0	7705	7.21E-03	0.520	0	14.9	54.8		
		37	14.0	1.00	l	7999	0	0	223	0	7705	7.21E-03	0.520	0	14.9	54.8		
		38	30.0	1.00	l	7999	0	0	223	0	7705	7.21E-03	0.520	0	14.9	54.8		
		38a	33.5	1.00	l	1.08E+04	0	0	1038	0	9700	7.21E-03	0.520	0	14.9	55.1		
g/l separation <1>		percentage of input in vapor phase			:		0	100	0	100	0	0	100	100	99.0	0		
		percentage of input in liquid phase			:		100	0	100	0	100	100	0	0	1.00	100		

	Comments	Streams	Temp [C]	P, atm	Phase	Total Flow	Acrylic acid	Oxygen	Acrolein	Propylene	Water	Acetic acid	Formaldehyde	Nitrogen	Acetaldehyde	Ethylhexanol, 2	Steam	Water
		Boiling Temperature (Tb) [oC]			:		139	-183	56.9	-47.7	99.9	118	-19.2	-194	20.9	183		
Waste		40	25.0	1.00	g	-15.3	0	0	0	0	0	0	-0.520	0	-14.7	0	0	0
		41	33.5	1.00	l	1.08E+04	0	0	1038	0	9700	7.21E-03	0	0	0.149	55.1		
		42	33.5	1.00	l	1.08E+04	0	0	1038	0	9700	7.21E-03	0	0	0.149	55.1		
	Feed	42	33.5	1.00	l		0	0	1038	0	9700	7.21E-03	0	0	0.149	55.1		
		streamphase					l	g	l	g	l	l	g	g	g	l		
Di <4>		percentage of input in distillate			:		0	100	97.0	100	10.0	0.100	100	100	100	0.100		
		percentage of input in bottoms			:		100	0	3.00	0	90.0	99.9	0	0	0	99.9		
		Boiling Temperature (Tb) [oC]			:		139	-183	56.9	-47.7	99.9	118	-19.2	-194	20.9	183		
	Distillate	43	57.0	1.00	l	1977	0	0	1007	0	970	7.21E-06	0	0	0.149	0.0551		
		streamphase					l	g	l	g	l	l	g	g	g	l		
	Bottoms	46	57.0	1.00	l	8816	0	0	31.1	0	8730	7.20E-03	0	0	0	55.1		
		streamphase					l	g	l	g	l	l	g	g	g	l		
		43	57.0	1.00	l	1977	0	0	1007	0	970	7.21E-06	0	0	0.149	0.0551		
		44	57.0	1.00	l	1977	0	0	1007	0	970	7.21E-06	0	0	0.149	0.0551		
	Feed	44	57.0	1.00	l	1977	0	0	1007	0	970	7.21E-06	0	0	0.149	0.0551		
		streamphase					l	g	l	g	l	l	g	g	g	l		
Di <5>		percentage of input in distillate			:				98.8		0.500	0			100	0		
		percentage of input in bottoms			:		100	100	1.20	100	99.5	100	100	100	0	100		
		Boiling Temperature (Tb) [oC]			:		139	-183	56.9	-47.7	99.9	118	-19.2	-194	20.9	183		
	Distillate	45	57.0	1.00	l	1000	0	0	995	0	4.85	0	0	0	0.149	0		
		streamphase							l		l				g			
	Bottoms	45c	57.0	1.00	l	977	0	0	12.1	0	965	7.21E-	0	0	0	0.0551		

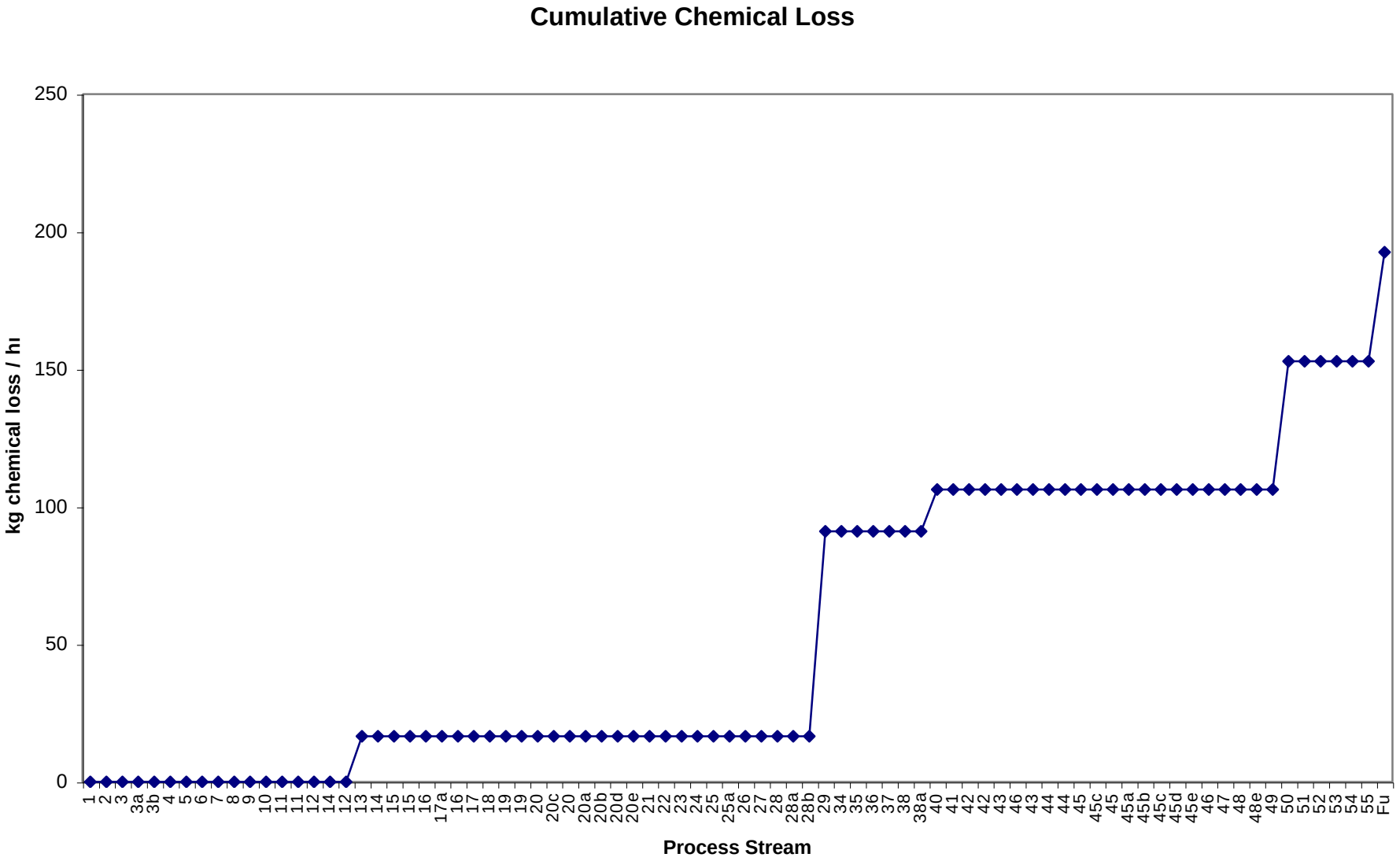
	Comments	Streams	Temp [C]	P, atm	Phase	Total Flow	Acrylic acid	Oxygen	Acrolein	Propylene	Water	Acetic acid	Formaldehyde	Nitrogen	Acetaldehyde	Ethylhexanol, 2	Steam	Water
												06						
		streamphase							l		l	l				l		
		45	57.0	1.00	l	1000	0	0	995	0	4.85	0	0	0	0.149	0		
		45a	57.0	1.00	l	1000	0	0	995	0	4.85	0	0	0	0.149	0		
Main product		45b	25.0	1.00	l	-1000	0	0	-995	0	-4.85	0	0	0	-0.149	0	0	0
		45c	57.0	1.00	l	977	0	0	12.1	0	965	7.21E-06	0	0	0	0.0551		
		45d	57.0	1.00	l	977	0	0	12.1	0	965	7.21E-06	0	0	0	0.0551		
		45e	25.0	1.00	l	977	0	0	12.1	0	965	7.21E-06	0	0	0	0.0551		
		46	57.0	1.00	l	8816	0	0	31.1	0	8730	7.20E-03	0	0	0	55.1		
		48	25.0	1.00	l	8816	0	0	31.1	0	8730	7.20E-03	0	0	0	55.1		
		48e	25.0	1.00	l	9793	0	0	43.2	0	9695	7.21E-03	0	0	0	55.1		
Decanter 1		percentage in oil phase			:		99.0	0	5.00	99.0	1.00	99.0	50.0	0	90.0	90.0		
		percentage in aqueous phase			:		1.00	100	95.0	1.00	99.0	1.00	50.0	100	10.0	10.0		
		49	25.0	1.00	l	9645	0	0	41.1	0	9598	7.21E-05	0	0	0	5.51		
Waste		50	25.0	1.00	l	-9645	0	0	-41.1	0	-9598	-7.21E-05	0	0	0	-5.51	0	0
		51	25.0	1.00	l	149	0	0	2.16	0	97.0	7.14E-03	0	0	0	49.6		
Input		53	25.0	1.00	l	8009					8000					9.00		
		54	28.8	1.00	l	8642	0	0	2.16	0	8097	7.14E-03	0	0	0	543		
		55	2.00	1.00	l	8642	0	0	2.16	0	8097	7.14E-03	0	0	0	543		
		Product purity (%)				0.995												
		Main product				Acrolein												
		Overall Rxn coefficients						-1.00	1.00	-1.00	1.00							
		Total yield of process (from reactant)						46.3	NA	76.3	NA							
Waste		Fugitive Losses (Total)			g	-79.7	0	0	-19.90	-19.2	0	-0.343	-0.137	0	-0.0753	0	0	0
		Input Sum				1.59E+04	0	1226	0	960	9644	0	0	4039	0	9.00		
		Fugitive Replacement of				19.2		0		19.2								

Griffing and Overcash, Chemical Life Cycle Database, www.environmentalclarity.com, 1999-present.

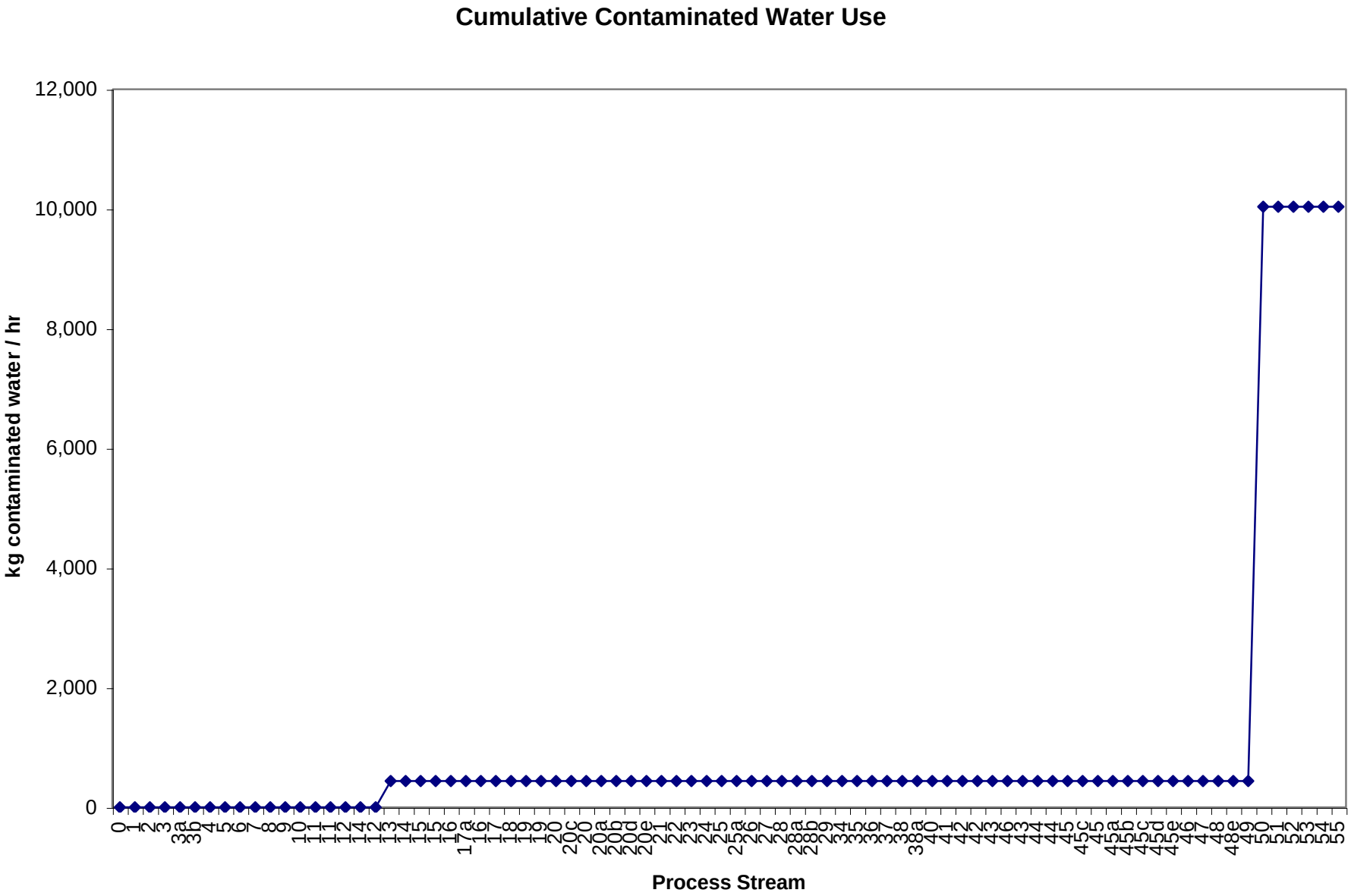
	Comments	Streams	Temp [C]	P, atm	Phase	Total Flow	Acrylic acid	Oxygen	Acrolein	Propylene	Water	Acetic acid	Formaldehyde	Nitrogen	Acetaldehyde	Ethylhexanol, 2	Steam	Water
		Reactants																
		Total Input (Input + Fugitive Replacement)				1.59E+04	0	1226	0	979	9644	0	0	4039	0	9.00		
		Product Sum				1196	147	0	995	0	5.29	33.9	0	0	0.149	14.9		
		Main product flow				1000	0	0	995	0	4.85	0	0	0	0.149	0		
		Net Input				-96.7												
Input		C1	20.0	1.00	l	3.81E+04												3.81E+04
Cooling out		C2	50.0	1.00	l	-3.81E+04												-3.81E+04
Input		C3	20.0	1.00	l	7669												7669
Cooling out		C4	50.0	1.00	l	-7669												-7669
Input		C5	20.0	1.00	l	6873												6873
Cooling out		C6	50.0	1.00	l	-6873												-6873
Input		C7	20.0	1.00	l	1351												1351
Cooling out		C8	50.0	1.00	l	-1351												-1351
Input		C9	20.0	1.00	l	1281												1281
Cooling out		C10	50.0	1.00	l	-1281												-1281
Input		C11	20.0	1.00	l	228												228
Cooling out		C12	50.0	1.00	l	-228												-228
Input		C13	20.0	1.00	l	2.64E+04												2.64E+04
Cooling out		C14	50.0	1.00	l	-2.64E+04												-2.64E+04
Input		C17	20.0	1.00	l	5.68E+04												5.68E+04
Cooling out		C18	50.0	1.00	l	-5.68E+04												-5.68E+04
Input		C19	20.0	1.00	l	9593												9593
Cooling out		C20	50.0	1.00	l	-9593												-9593
Input		C21	20.0	1.00	l	470												470
Cooling out		C22	50.0	1.00	l	-470												-470
Input		C23	20.0	1.00	l	6399												6399
Cooling out		C24	50.0	1.00	l	-6399												-6399
Input		C25	20.0	1.00	l	7968												7968
Cooling out		C26	50.0	1.00	l	-7968												-7968
Input		C27	20.0	1.00	l	882												882
Cooling out		C28	50.0	1.00	l	-882												-882
Input		S1	207	1.00	g	2568											2568	
Steam out		S2	207	1.00	l	--2568											-2568	

	Comments	Streams	Temp [C]	P, atm	Phase	Total Flow	Acrylic acid	Oxygen	Acrolein	Propylene	Water	Acetic acid	Formaldehyde	Nitrogen	Acetaldehyde	Ethylhexanol, 2	Steam	Water
Input		S3	207	1.00	g	615											615	
Steam out		S4	207	1.00	l	-615											-615	
Input		S5	207	1.00	g	139											139	
Steam out		S6	207	1.00	l	-139											-139	
Input		S7	207	1.00	g	135											135	
Steam out		S8	207	1.00	l	-135											-135	
Input		S9	207	1.00	g	5749											5749	
Steam out		S10	207	1.00	l	-5749											-5749	
Input		S11	207	1.00	g	329											329	
Steam out		S12	207	1.00	l	-329											-329	
Input		S13	207	1.00	g	590											590	
Steam out		S14	207	1.00	l	-590											-590	
Input		S15	207	1.00	g	867											867	
Steam out		S16	207	1.00	l	-867											-867	

Graph of Cumulative Chemical Losses through Manufacturing Process

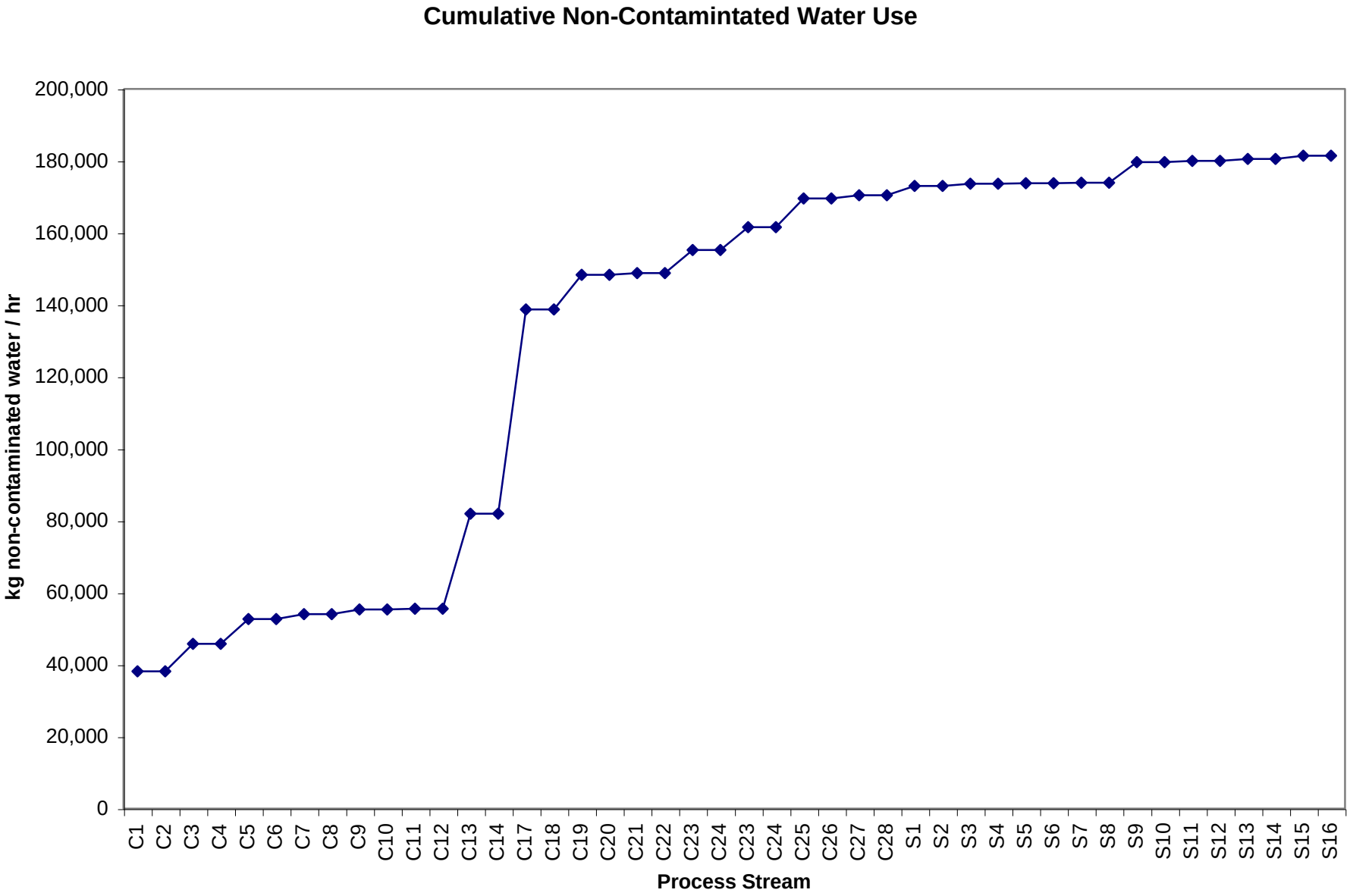


Graph of Cumulative Contaminated Water Use / Emission through Manufacturing Process



Griffing and Overcash, Chemical Life Cycle Database, www.environmentalclarity.com, 1999-present.

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



Griffing and Overcash, Chemical Life Cycle Database, www.environmentalclarity.com, 1999-present.

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	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]
Cmp1	Compressor 1	54.6	54.6		E	R1	Reactor 1	-5631	-5631	350	0.600	-3379	-3379
Cmp2	Compressor 2	285	340		E	Hx2	Heat exchanger 2	-1133	-6763	350	0.600	-680	-4058
Cmp3	Compressor 3	462	802		E	Di1	Distillation condenser 1	-1015	-7778	98.9	0.250	-254	-4312
P1	Pump 1	0.0968	802		E	Di2	Distillation condenser 2	-199	-7978	117	0.250	-49.9	-4362
Hx1	Heat exchanger 1	4174	4976	100	S	Di3	Distillation condenser 3	-189	-8167	138	0.250	-47.3	-4409
P2	Pump 2	1.12E-03	4976		E	Hx3	Heat exchanger 3	-33.6	-8201	139	0.250	-8.40	-4417
Di1	Distillation reboiler 1	1000	5976	98.9	S	Hx5	Heat exchanger 5	-69.4	-8270	57.0	0	0	-4417
P3	Pump 3	3.72E-05	5976		E	Hx6	Heat exchanger 6	-1177	-9447	57.0	0	0	-4417
P4	Pump 4	2.88E-04	5976		E	Di4	Distillation condenser 4	-8383	-17830	55.9	0	0	-4417
Di2	Distillation reboiler 2	226	6203	117	S	Di5	Distillation condenser 5	-1417	-19246	55.9	0	0	-4417
P5	Pump 5	1.11E-07	6203		E								
P6	Pump 6	2.34E-04	6203		E								
Di3	Distillation reboiler 3	219	6422	138	S								
P7	Pump 7	7.87E-03	6422		E								
P8	Pump 8	0.0338	6422		E								
P9	Pump 9	3.63E-04	6422		E								
P10	Pump 10	2.01	6424		E								
P11	Pump 11	0.0649	6424		E								
Ref1	Refrigerator elect. 1	927	7351	0	E								
P12	Pump 12	0.604	7351		E								
P13	Pump 13	0.219	7351		E								
Di4	Distillation reboiler 4	9343	1.67E+04	55.9	S								
P14	Pump 14	2.41E-03	1.67E+04		E								
P15	Pump 15	0.696	1.67E+04		E								

P16	Pump 16	8.59E-03	1.67E+04		E									
P17	Pump 17	0.160	1.67E+04		E									
Ref2	Refrigerator elect. 2	311	1.70E+04	0	E									
Hx4	Heat exchanger 4	535	1.75E+04	30.0	S									
:	Washer 1	959	1.85E+04	0	S									
Di5	Distillation reboiler 5	1409	1.99E+04	55.9	S									
P18	Pump 18	0.0693	1.99E+04		E									
P19	Pump 19	0.564	1.99E+04		E									
	Potential recovery	-4417	1.55E+04											
	Net energy		1.55E+04				Potential recovery:							-4417
	Electricity	2045	E	[MJ/hr]										
	DowTherm	0	D	[MJ/hr]										
	Heating steam	1.79E+04	S	[MJ/hr]										
	Direct fuel use	0	F	[MJ/hr]										
	Heating natural gas	0	G	[MJ/hr]										
	Energy input requirement	1.99E+04		[MJ/hr]										
	Cooling water	-1.92E+04		[MJ/hr]										
	Cooling refrigeration			[MJ/hr]										
	Potential heat recovery	-4417		[MJ/hr]										
	Net energy	1.55E+04		[MJ/hr]										

Graph of Cumulative Energy Requirements