Pd on carbon (activated carbon impregnated with Pd)

CONTENTS OF FACTORY GATE TO FACTORY GATE

LIFE CYCLE INVENTORY SUMMARY

Chemistry

Adsorption reactions:

$$PdCl_2 + 2NaCl \rightarrow Na_2PdCl_4 \quad (1)$$
$$Na_2PdCl_4 + H_2O_2 \rightarrow Na_2PdCl_4(OH)_2 \quad (2)$$
$$Na_2PdCl_4(OH)_2 + 2NaOH + C \rightarrow C\text{-}Pd(OH)_4 + 4NaCl \quad (3)$$

Net reaction

$$PdCl_2 + H_2O_2 + 2NaOH + C \rightarrow C\text{-}Pd(OH)_4 + 2NaCl \quad (4)$$

palladium chloride + hydrogen peroxide + sodium hydroxide + activated carbon → adsorbed catalyst hydroxide + sodium chloride

Reduction reactions:

$$C\text{-}Pd(OH)_4 + 4e^- \rightarrow C\text{-}Pd + 4OH^- \quad (5)$$
$$CH_2O + H_2O \rightarrow CO_2 + 4H^+ + 4e^- \quad (6)$$

Net:

$$C\text{-}Pd(OH)_4 + CH_2O \rightarrow C\text{-}Pd + CO_2 + 3H_2O \quad (7)$$

adsorbed palladium hydroxide+ formaldehyde → adsorbed palladium + carbon dioxide + water

Notes:

The rxn chemistry varies in the literature. This represents one option. The reduction reaction (7) is inferred.

Process Summary

Literature

Several supports are commonly used for PGMs. When carbon is used as a support, it is in one of three forms, activated carbon, carbon black, or graphite. The type of support typically depends on the desired pore structure for a given application. In the preparation stage, the process is similar regardless of the support type. Therefore, any one of the three supports could be substituted in this GTG LCI report.

Palladium can either be deposited on the surface of a carbon sphere (called egg-shell morphology) or impregnated within the carbon. Again, the method depends on the final application. The eggshell catalysts do not last as long due to the limited surface area, but provide better reaction rates for diffusion-limited processes. Eggshell catalysts are manufactured by applying colloidal metal to the carbon. Impregnated catalysts are formed by contacting a suspension of activated carbon (in water) with an ionic palladium species such as $[Pd(OH)_4]^{2-}$ (Auer, 1998).

When $PdCl_2$ is added directly to most carbon supports, the palladium is immediately deposited as a shiny film. Catalysts formed in this way generally have a low activity (U.S. 3,138,560). Therefore, various pretreatments of $PdCl_2$ and the catalyst have been studied in order to increase catalyst activity. Several patents (US 6,963,016; US 4,415,479; US 6,624,109; US 5,753,583) discuss methods producing catalysts with high activity for specific reactions. A more generic process is discussed in U.S. 2,857,337 and U.S. 3,138,560. In these patents, the $PdCl_2$ is pre-treated with either H_2O_2 or $NaHCO_3$ and either NaCl or HCl. In these cases, the Pd is thought to be deposited as $Pd(OH)_2$ (US 2,857,337) or $Pd(OH)_4$ (US 3,138,560), which is consistent with Auer (1998) and Stiles (1983). In this GTG LCI report, we use NaCl and H_2O_2, as described in the chemistry section.

A solution of palladium chloride in water is prepared. The mass percentage of Pd is given as 1% (Stiles, 1983), 0.25% (US 3,138,560), and 2% (US 2,857,337). A 1% solution is used in this GTG report. NaCl and H_2O_2 are added. We use a 5% stoichiometric excess of NaCl (US 3,138,560 starts with Na_2PdCl_4). A 50% excess of H_2O_2 is used as given by U.S. 3,138,560.

A slurry of activated carbon solids in water is prepared separately. Stiles (1983) writes that 1 to 5% carbon is used. US 2,857,337 gives a 10% carbon solution. The activated carbon is generally pre-treated with an alkali hydroxide wash if metal content will be higher than 5% or the carbon is particularly basic. We used a 5%NaOH solution to pretreat a 3 wt% carbon solution, followed by rinsing and drying of the carbon.

Stiles (1983) teaches that both the carbon and metal solutions are heated to 50ºC and combined. In US 2,857,337, the streams are combined, and then the solution is heated to 90-95ºC for impregnation. US 3,138,560 makes no mention of temperature. We combine the streams and heat to 70ºC in this GTG LCI. Sodium hydroxide is added prior to heating 1.1 times the stoichiometric requirement for reaction (3).

Once the activated carbon is loaded with palladium (as $Pd(OH)_4$), various process descriptions diverge. In US 3,138,560, the catalyst is simply washed and dried. No mention is made of reducing the palladium in the examples. Both Stiles (1983) and US 2,857,337 discuss reduction with either formaldehyde or hydrogen. In US 2,857,337, the reduction is performed by adding a formaldehyde solution to the hot catalyst solution. Stiles (1983) recommends first washing the catalyst with demineralized water prior to reduction with formaldehyde (10X stoichiometric quantity). In this GTG LCI, we include a wash, followed by a reduction with formaldehyde, another series of washes, and finally the catalyst is dried. Catalyst drying is at 80 – 200ºC (Stiles, 1983). The initial drying, prior to reduction is at 120 oC, and the final product is dried at 100ºC.

LCI design

Palladium dichloride, sodium chloride, water and hydrogen peroxide are mixed. Activated carbon is pre-treated by rinsing with NaOH in water (5%). In the wash, 0.33 kg of HCl was present for every 1 kg of carbon. A recycle was used, so that 0.11 kg HCl was consumed per kg of activated carbon. After pre-treatment, the carbon was dried, and water was added to make a 3.1% activated carbon slurry.

The pretreated carbon is filtered, rinsed, and dried at 120 ºC. Water and sodium hydroxide are added and the carbon and palladium streams are combined in an adsorption reactor. Palladium adsorbs as $Pd(OH)_4$ at 70 ºC. The palladium loaded carbon is then filtered (the liquid is discarded) and rinsed. Formaldehyde is added at 10 times the stoichiometric requirement to reduce the $Pd(OH)_4$ to Pd. Carbon dioxide and water vapor leave the reactor, and are cooled and treated as waste. The reduced catalyst is filtered (liquid is discarded), rinsed, and dried at 100ºC.

Comments on design assumptions

The mass efficiency of this report is high (99% of yield based on Pd). The energy is dominated by Reactor 1 and the Dryers. The largest energy contribution (reactor) is determined by the percent carbon and temperature in the adsorption reactor. These are between 1 and 5% (in the literature) and between 50 and 90ºC. We used 3% and 70ºC.

The reaction chemistry varies widely in the literature.

Critical parameters

Conversion / Yield information from both reactors					
		Conversion of or Yield from palladium chloride	Conversion of or Yield from sodium hydroxide	Conversion of or Yield from hydrogen peroxide	Conversion of or Yield from Formaldehyde
Total conversion in reactor 1: (% of reactant entering the process that reacts)	From mass balance	99	33.6	94.3	
Total per pass conversion in reactor 1: (% of reactant entering the reactor that reacts)	From mass balance	99	60.8	94.3	
Total yield of reactor 1: (% yield $Pd(OH)_4$ produced in the reactor based on reactant input to process)	From mass balance	99	60.8	94.3	
Total conversion in reactor 2: (% of reactant entering the process that reacts)	From mass balance				10
Total per pass conversion in reactor 2: (% of reactant entering the reactor that reacts)	From mass balance				10
Total yield of reactor 2:	From mass				10

(% yield produced in the reactor based on reactant input to process)	balance				
Total yield of Process: (% yield produced by the overall process based on reactant input to process)	From mass balance	99	34	94	10
Notes: Per pass conversion is higher than total conversion for NaOH in reactor 1, because some NaOH enters the process elsewhere, and is not used in this reactor.					

Product purity			
	Pd on C 10%		Comments
Used here	99.9		10 kg Pd, 899 kg C, 1 kg water

Summary of LCI Information

Inputs					
Input UID	Input Name	Input Flow	Input purity	Units	Comments
7647-10-1	palladium chloride	168		[kg/hr]	
UIDActivatedCarbon	activated carbon	900		[kg/hr]	
50-00-0	Formaldehyde	284		[kg/hr]	
1310-73-2	Sodium hydroxide	224		[kg/hr]	
7722-84-1	Hydrogen peroxide	33.9		[kg/hr]	
7647-14-5	Sodium chloride	117		[kg/hr]	
	Total	1726		[kg/hr]	
Non-reacting inputs					
UID	Name	Flow	Purity	Units	Comments
7732-18-5	Water	6.75e+4		[kg/hr]	
	Total	6.75e+4		[kg/hr]	
Ancillary inputs					
UID	Name	Flow	Purity	Units	Comments
No ancillary inputs					
Products					
Product UID	Product Name	ProductFlow	Purity	Units	Comments
UIDPdOnC10	palladium on carbon (10%)	1000	99.9	[kg/hr]	100 kg Pd on 899kg carbon
	Total	1000		[kg/hr]	
Benign Outflows					
UID	Name	Flow	Purity	Units	Comments
7732-18-5	Water	6.75e+4		[kg/hr]	
	Total	6.75e+4		[kg/hr]	

Chemical Emissions							
Emission UID	Emission Name	Gas Flow	Liquid Flow	Solid Flow	Solvent Flow	Units	Comments
124-38-9	Carbon dioxide	39.5	1.98	0	0	[kg/hr]	
1310-73-2	Sodium hydroxide	0	148	0	0	[kg/hr]	
50-00-0	Formaldehyde	1.41	254	0	0	[kg/hr]	
7647-10-1	palladium chloride	0	1.68	0	0	[kg/hr]	
7647-14-5	Sodium chloride	0	227	0	0	[kg/hr]	
UIDActivatedCarbon	activated carbon	0	1.000	0	0	[kg/hr]	
Totals		41.0	634	0	0	[kg/hr]	

Mass Balance		
Total inputs	6.92e+4	
Total outflows	6.92e+4	
Net input	1.94	

Energy use			
Energy type	Amount	Comments	
electricity	31.4	[MJ/hr]	
heating steam	1.45e+4	[MJ/hr]	
Net input requirement	1.45e+4	[MJ/hr]	Net of energies input to system
cooling water	-1.25e+4	[MJ/hr]	
potential recovery	-3115	[MJ/hr]	
Net energy	1.14e+4	[MJ/hr]	Net input requirement - potential recovery

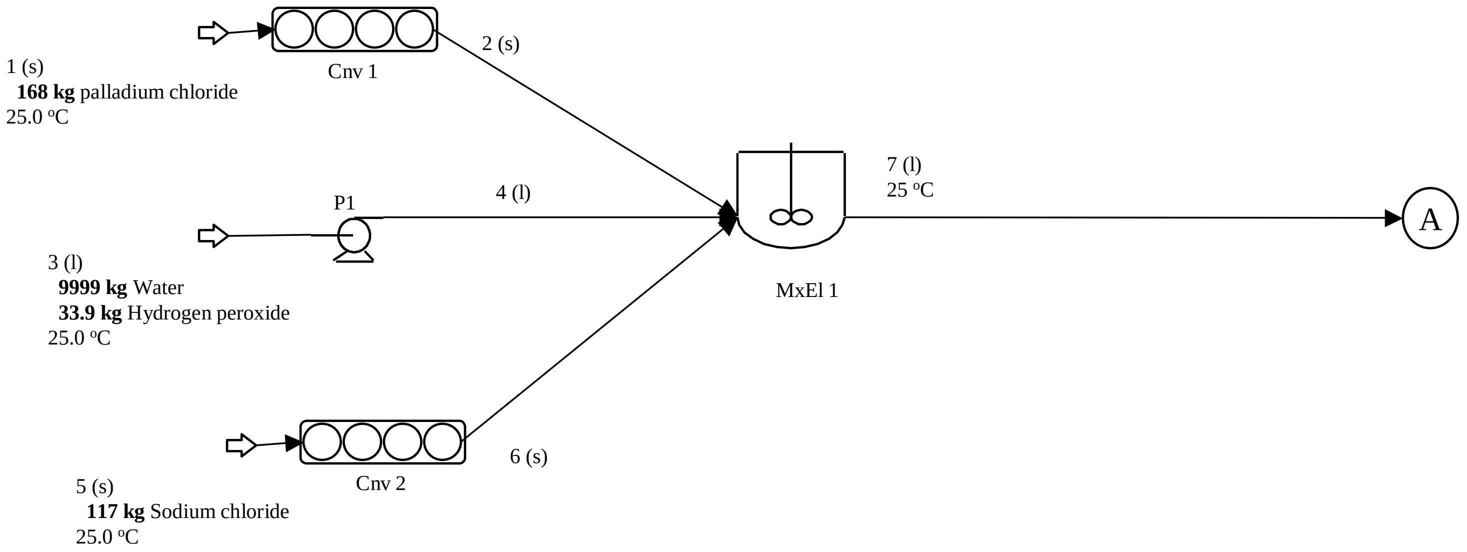
Process Diagram Interpretation Sheet

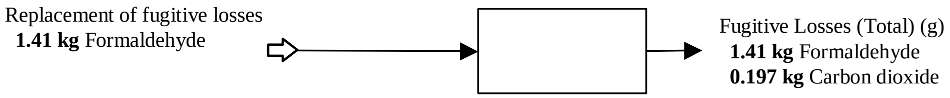
1) As much as possible, standard symbols are used for all unit processes.
2) Only overall input and output chemicals are labeled on these diagrams. All intermediate information is given on the attached Process Mass Balance sheet
3) The physical state of most streams is shown (gas, g; liquid, l; solid, 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

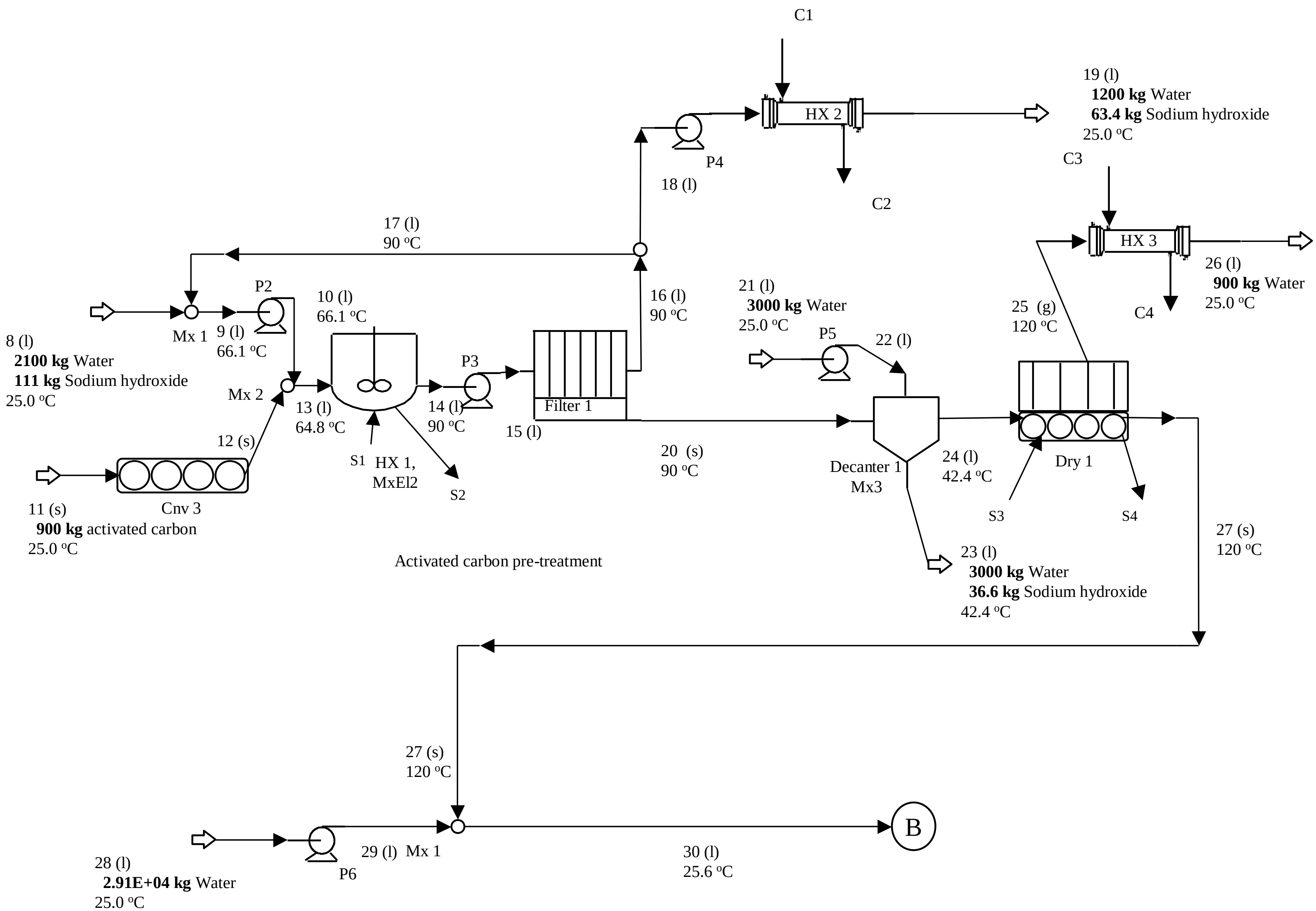
For most streams, the temperature and pressure are shown, if the pressures are greater than 1 atm

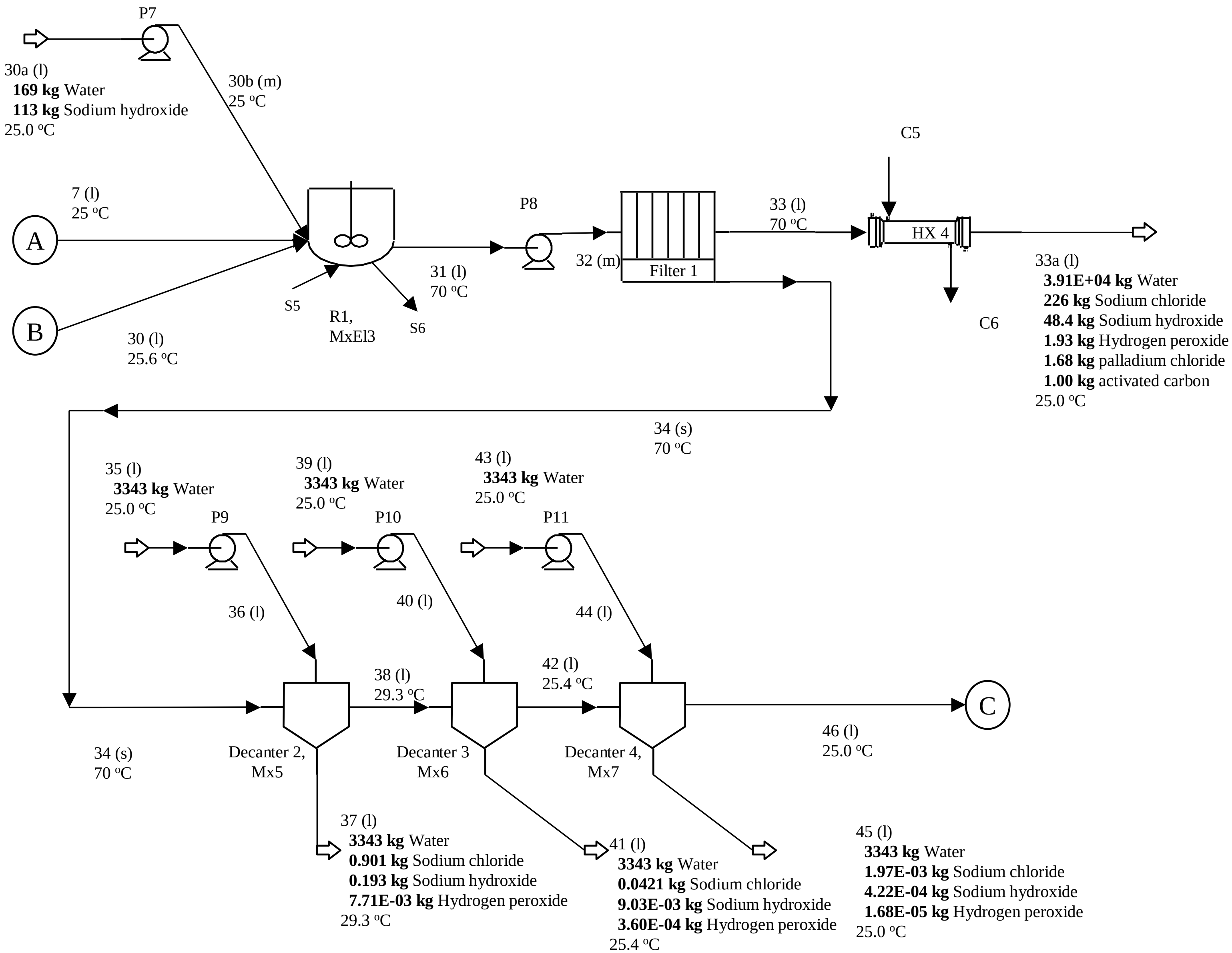
Process Diagram or Boundary of LCI

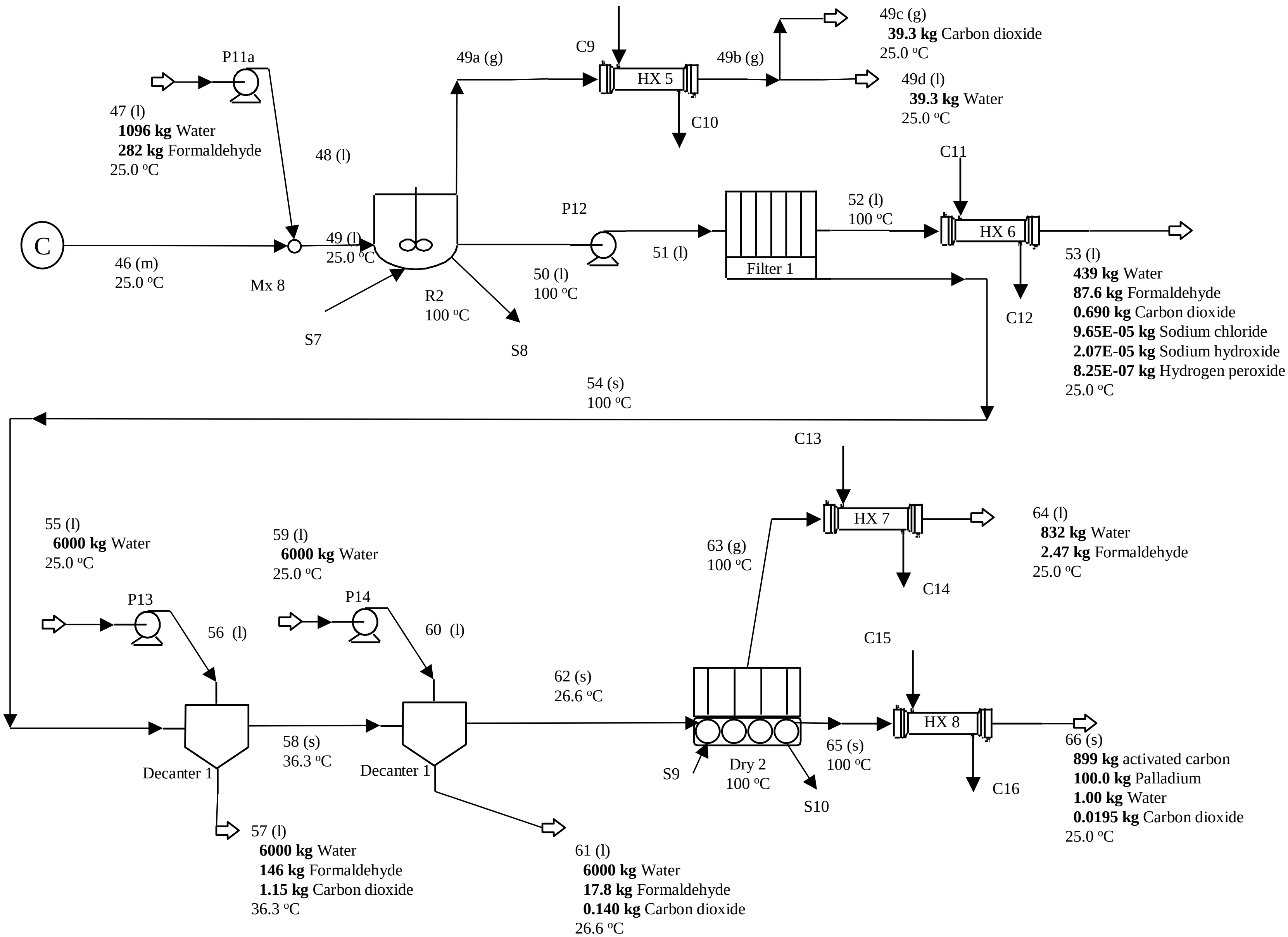
Steam enters the process as a gas at 207 ºC and leaves as a liquid at 207 ºC. Cooling water enters at 20 ºC and leaves at 50 ºC. Unless otherwise indicated, all processes are at 1 atm and 25ºC.






C1
19 (l)
1200 kg Water
63.4 kg Sodium hydroxide
25.0 ºC
HX 2
P4
18 (l)
C2
C3
HX 3
17 (l)
90 ºC
26 (l)
900 kg Water
25.0 ºC
P2
10 (l)
66.1 ºC
16 (l)
90 ºC
21 (l)
3000 kg Water
25.0 ºC
25 (g)
120 ºC
C4
8 (l)
2100 kg Water
111 kg Sodium hydroxide
25.0 ºC
Mx 1
9 (l)
66.1 ºC
P5
22 (l)
P3
Mx 2
13 (l)
64.8 ºC
14 (l)
90 ºC
Filter 1
15 (l)
12 (s)
S1
HX 1,
MxEl2
S2
20 (s)
90 ºC
Decanter 1
Mx3
24 (l)
42.4 ºC
Dry 1
S3
S4
11 (s)
900 kg activated carbon
25.0 ºC
Cnv 3
27 (s)
120 ºC
23 (l)
3000 kg Water
36.6 kg Sodium hydroxide
42.4 ºC
Activated carbon pre-treatment
27 (s)
120 ºC
28 (l)
2.91E+04 kg Water
25.0 ºC
P6
29 (l)
Mx 1
30 (l)
25.6 ºC
B


P7
30a (l)
169 kg Water
113 kg Sodium hydroxide
25.0 ºC
30b (m)
25 ºC
7 (l)
25 ºC
A
B
30 (l)
25.6 ºC
S5
R1,
MxEl3
S6
31 (l)
70 ºC
P8
32 (m)
Filter 1
33 (l)
70 ºC
C5
HX 4
C6
33a (l)
3.91E+04 kg Water
226 kg Sodium chloride
48.4 kg Sodium hydroxide
1.93 kg Hydrogen peroxide
1.68 kg palladium chloride
1.00 kg activated carbon
25.0 ºC
34 (s)
70 ºC
35 (l)
3343 kg Water
25.0 ºC
P9
39 (l)
3343 kg Water
25.0 ºC
P10
43 (l)
3343 kg Water
25.0 ºC
P11
36 (l)
40 (l)
44 (l)
38 (l)
29.3 ºC
42 (l)
25.4 ºC
C
46 (l)
25.0 ºC
34 (s)
70 ºC
Decanter 2,
Mx5
Decanter 3
Mx6
Decanter 4,
Mx7
37 (l)
3343 kg Water
0.901 kg Sodium chloride
0.193 kg Sodium hydroxide
7.71E-03 kg Hydrogen peroxide
29.3 ºC
41 (l)
3343 kg Water
0.0421 kg Sodium chloride
9.03E-03 kg Sodium hydroxide
3.60E-04 kg Hydrogen peroxide
25.4 ºC
45 (l)
3343 kg Water
1.97E-03 kg Sodium chloride
4.22E-04 kg Sodium hydroxide
1.68E-05 kg Hydrogen peroxide
25.0 ºC



P11a
47 (l)
1096 kg Water
282 kg Formaldehyde
25.0 ºC
48 (l)
49a (g)
C9
HX 5
49b (g)
C10
49c (g)
39.3 kg Carbon dioxide
25.0 ºC
49d (l)
39.3 kg Water
25.0 ºC
C
46 (m)
25.0 ºC
Mx 8
49 (l)
25.0 ºC
R2
100 ºC
S7
S8
P12
50 (l)
100 ºC
51 (l)
Filter 1
52 (l)
100 ºC
C11
HX 6
C12
53 (l)
439 kg Water
87.6 kg Formaldehyde
0.690 kg Carbon dioxide
9.65E-05 kg Sodium chloride
2.07E-05 kg Sodium hydroxide
8.25E-07 kg Hydrogen peroxide
25.0 ºC
54 (s)
100 ºC
C13
HX 7
C14
63 (g)
100 ºC
64 (l)
832 kg Water
2.47 kg Formaldehyde
25.0 ºC
55 (l)
6000 kg Water
25.0 ºC
P13
56 (l)
59 (l)
6000 kg Water
25.0 ºC
P14
60 (l)
62 (s)
26.6 ºC
Decanter 1
58 (s)
36.3 ºC
Decanter 1
57 (l)
6000 kg Water
146 kg Formaldehyde
1.15 kg Carbon dioxide
36.3 ºC
61 (l)
6000 kg Water
17.8 kg Formaldehyde
0.140 kg Carbon dioxide
26.6 ºC
S9
Dry 2
100 ºC
S10
65 (s)
100 ºC
C15
HX 8
C16
66 (s)
899 kg activated carbon
100.0 kg Palladium
1.00 kg Water
0.0195 kg Carbon dioxide
25.0 ºC

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	Water	Palladium	palladium chloride	activated carbon	Pd(OH)4 on C	Formaldehyde	Carbon dioxide	Sodium hydroxide	Hydrogen peroxide	Sodium chloride	Steam	Water
		0		1.00		0	0	0	0	0	0	0	0	0	0	0	0	0
Input		1	25.0	1.00	s	168			168									
		2	25.0	1.00	s	168	0	0	168	0	0	0	0	0	0	0		
Input		3	25.0	1.00	l	1.00E+04	9999								33.9			
		4	25.0	1.00	l	1.00E+04	9999	0	0	0	0	0	0	0	33.9	0		
Input		5	25.0	1.00	s	117										117		
		6	25.0	1.00	s	117										117		
		7	25.0	1.00	l	1.03E+04	9999	0	168	0	0	0	0	0	33.9	117		
Input	0.0000 % NaOH	8	25.0	1.00	l	2211	2100							111				
		Stream 17:Recycle input				3790	3600							190				
		Stream 17:Recycle calculated				3790	3600	0	0	0	0	0	0	190	0	0		
		Stream 17:Recycle residue				-0.105	0	0	0	0	0	0	0	-0.105	0	0		
		9	66.1	1.00	l	6001	5700	0	0	0	0	0	0	301	0	0		
		10	66.1	1.00	l	6001	5700	0	0	0	0	0	0	301	0	0		
Input		11	25.0	1.00	s	900				900								
		12	25.0	1.00	s	900				900								
		13	64.8	1.00	l	6901	5700	0	0	900	0	0	0	301	0	0		
		14	90.0	1.00	l	6901	5700	0	0	900	0	0	0	301	0	0		
		15	90.0	1.00	l	6901	5700	0	0	900	0	0	0	301	0	0		
		16	90.0	1.00	l	5053	4800							253				
		17	90.0	1.00	l	3790	3600							190				
		18	90.0	1.00	l	1263	1200	0	0	0	0	0	0	63.4	0	0		
Waste		19	25.0	1.00	l	-1263	-1200	0	0	0	0	0	0	-63.4	0	0	0	0
		20	90.0	1.00	l	1848	900	0	0	900	0	0	0	47.5	0	0		
Input		21	25.0	1.00	l	3000	3000											
		22	25.0	1.00	l	3000	3000											
Waste		23	42.4	1.00	l	-3037	-3000	0	0	0	0	0	0	-36.6	0	0	0	0

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Water	Palladium	palladium chloride	activated carbon	Pd(OH)4 on C	Formaldehyde	Carbon dioxide	Sodium hydroxide	Hydrogen peroxide	Sodium chloride	Steam	Water
		24	42.4	1.00	l	1811	900	0	0	900	0	0	0	11.0	0	0		
		25	120	1.00	g	900	900											
Waste		26	25.0	1.00	l	-900	-900	0	0	0	0	0	0	0	0	0	0	0
		27	120	1.00	s	911	0	0	0	900	0	0	0	11.0	0	0		
Input		28	25.0	1.00	l	2.91E+04	2.91E+04											
		29	25.0	1.00	l	2.91E+04	2.91E+04							0				
	0.0000 % carbon	30	25.6	1.00	l	3.00E+04	2.91E+04	0	0	900	0	0	0	11.0	0	0		
Input		30a	25.0	1.00	l	282	169							113				
		30b	25.0	1.00	l	282	169							113				
R1	167	kg	palladium chloride			is converted in rxn 1 (99.0 % of reactor input)												
		kg				is lost in rxn 2												
		kg				is lost in rxn 3												
		Input to reactor			:	4.06E+04	3.93E+04	0	168	900	0	0	0	124	33.9	117		
		R1 Reaction Coefficient 1			:				-1.00		1.00			-2.00	-1.00	2.00		
		R1 Conversion 1 [kg/hr]			:	-0.0137			-167		164			-75.2	-32.0	110		
		R1 Conversion 1 [kgmol/hr]			:	0.940			-0.940		0.940			-1.88	-0.940	1.88		
		R1 Reaction Coefficient 2			:													
		R1 Conversion 2 [kg/hr]			:													
		R1 Conversion 2 [kgmol/hr]			:	Non-Number in input												
		R1 Reaction Coefficient 3			:													
		R1 Conversion 3 [kg/hr]			:													
		R1 Conversion 3 [kgmol/hr]			:													
		Flow out of reactor			:	4.06E+04	3.93E+04	0	1.68	900	164	0	0	48.6	1.94	227		
		Primary product			:	Palladium												
		Total conversion			:		-0	NA	99.0	-0	NA	-0	NA	33.6	94.3	-94.3		
		Per pass conversion			:		-0		99.0		NA			60.8	94.3	NA		
		Total yield from reactor			:			NA	99.0		NA			60.8	94.3	NA		
		31	70.0	1.00	l	4.06E+04	3.93E+04	0	1.68	900	164	0	0	48.6	1.94	227		

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Water	Palladium	palladium chloride	activated carbon	Pd(OH)4 on C	Formaldehyde	Carbon dioxide	Sodium hydroxide	Hydrogen peroxide	Sodium chloride	Steam	Water
		32	70.0	1.00	l	4.06E+04	3.93E+04	0	1.68	900	164	0	0	48.6	1.94	227		
		33	70.0	1.00	l	3.94E+04	3.91E+04		1.68	1.00				48.4	1.93	226		
Waste		33a	25.0	1.00	l	-3.94E+04	-3.91E+04	0	-1.68	-1.00	0	0	0	-48.4	-1.93	-226	0	0
		34	70.0	1.00	l	1228	164	0	7.03E-03	899	164	0	0	0.203	8.09E-03	0.946		
Input		35	25.0	1.00	l	3343	3343											
		36	25.0	1.00	l	3343	3343											
Waste		37	29.3	1.00	l	-3344	-3343	0	0	0	0	0	0	-0.193	-7.71E-03	-0.901	0	0
		38	29.3	1.00	l	1227	164			899	164			9.47E-03	3.78E-04	0.0442		
Input		39	25.0	1.00	l	3343	3343											
		40	25.0	1.00	l	3343	3343											
Waste		41	25.4	1.00	l	-3343	-3343	0	0	0	0	0	0	-9.03E-03	-3.60E-04	-0.0421	0	0
		42	25.4	1.00	l	1227	164			899	164			4.43E-04	1.77E-05	2.07E-03		
Input		43	25.0	1.00	l	3343	3343											
		44	25.0	1.00	l	3343	3343											
Waste		45	25.0	1.00	l	-3343	-3343	0	0	0	0	0	0	-4.22E-04	-1.68E-05	-1.97E-03	0	0
		46	25.0	1.00	l	1227	164			899	164			2.07E-05	8.25E-07	9.65E-05		
Input		47	25.0	1.00	l	1378	1096					282						
		48	25.0	1.00	l	1378	1096					282						
		49	25.0	1.00	l	2605	1260	0	0	899	164	282	0	2.07E-05	8.25E-07	9.65E-05		
R2	164	kg	Pd(OH)4 on C			is converted in rxn 1 (100 % of reactor input)												
		kg				is lost in rxn 2												
		kg				is lost in rxn 3												
		Input to reactor			:	2605	1260	0	0	899	164	282	0	2.07E-05	8.25E-07	9.65E-05		
		R2 Reaction Coefficient 1			:		3.00	1.00			-1.00	-1.00	1.00					
		R2 Conversion 1 [kg/hr]			:	-0.0282	50.7	100.0			-164	-28.2	41.3					
		R2 Conversion 1 [kgmol/hr]			:	2.82	2.82	0.940			-0.940	-0.940	0.940					

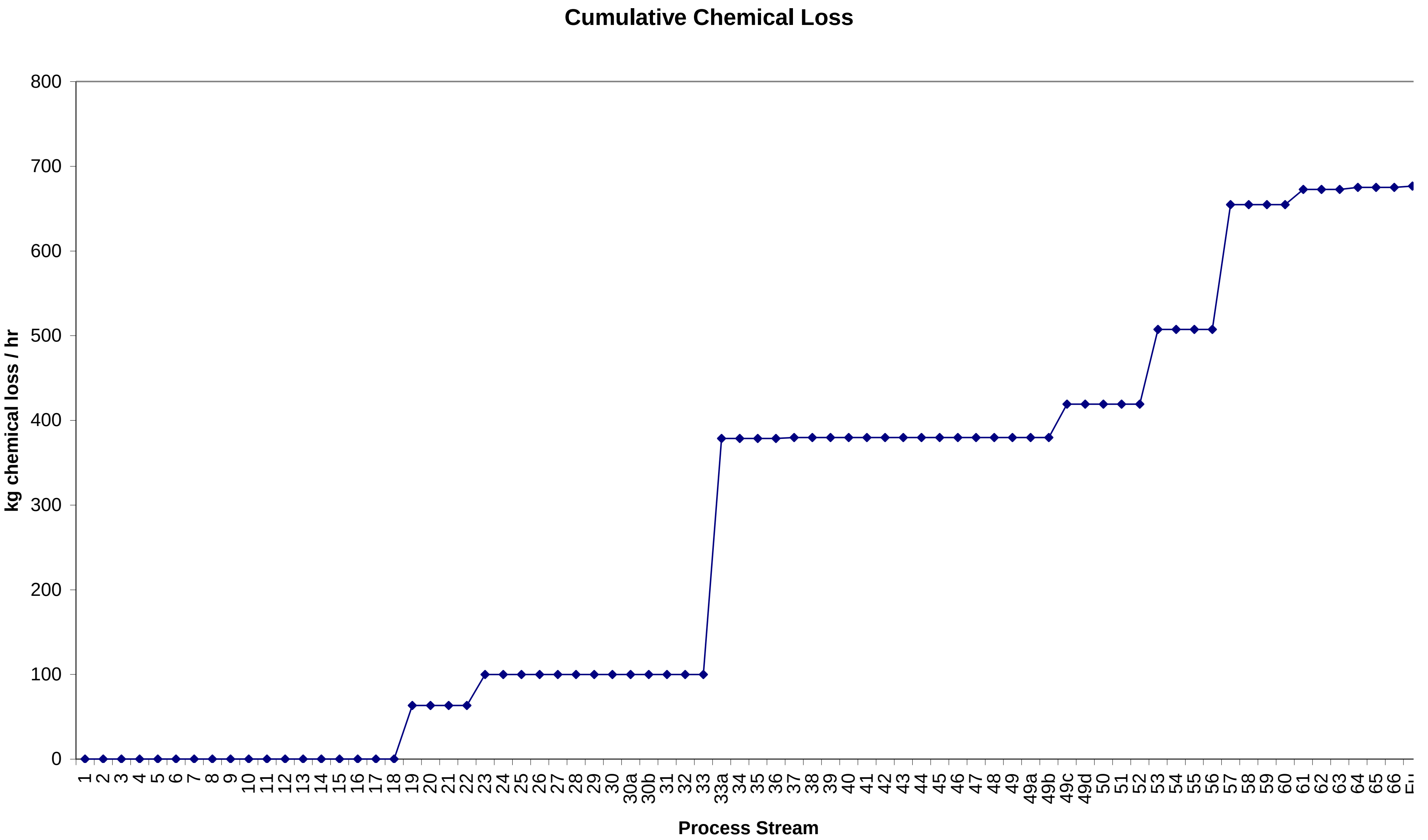
	Comments	Streams	Temp [C]	P	Phase	Total Flow	Water	Palladium	palladium chloride	activated carbon	Pd(OH)4 on C	Formaldehyde	Carbon dioxide	Sodium hydroxide	Hydrogen peroxide	Sodium chloride	Steam	Water
		R2 Reaction Coefficient 2			:													
		R2 Conversion 2 [kg/hr]			:													
		R2 Conversion 2 [kgmol/hr]			:	Non-Number in input												
		R2 Reaction Coefficient 3			:													
		R2 Conversion 3 [kg/hr]			:													
		R2 Conversion 3 [kgmol/hr]			:													
		Flow out of reactor			:	2605	1311	100.0	0	899	0	254	41.3	2.07E-05	8.25E-07	9.65E-05		
		Primary product			:	Palladium												
		Total conversion			:		-0.0752	NA	-0	-0	NA	10.0	NA	-0	-0	-0		
		Per pass conversion			:		NA	NA		-0	100	10.0	NA	-0	-0	-0		
		Total yield from reactor			:		NA	NA			100	100						
		49a	100	1.00	g	78.7	39.3						39.3					
		49b	25.0	1.00	l	78.7	39.3						39.3					
Waste		49c	25.0	1.00	g	-39.3	0	0	0	0	0	0	-39.3	0	0	0	0	0
Waste		49d	25.0	1.00	l	-39.3	-39.3	0	0	0	0	0	0	0	0	0	0	0
		50	100	1.00	l	2526	1271	100.0	0	899	0	254	2.00	2.07E-05	8.25E-07	9.65E-05		
		51	100	1.00	l	2526	1271	100.0	0	899	0	254	2.00	2.07E-05	8.25E-07	9.65E-05		
		52	100	1.00	l	527	439					87.6	0.690	2.07E-05	8.25E-07	9.65E-05		
Waste		53	25.0	1.00	l	-527	-439	0	0	0	0	-87.6	-0.690	-2.07E-05	-8.25E-07	-9.65E-05	0	0
		54	100	1.00	s	1999	833	100.0	0	899	0	166	1.31	0	0	0		
Input		55	25.0	1.00	l	6000	6000											
		56	25.0	1.00	l	6000	6000											
Waste		57	36.3	1.00	l	-6147	-6000	0	0	0	0	-146	-1.15	0	0	0	0	0
		58	36.3	1.00	s	1852	833	100.0	0	899	0	20.3	0.160	0	0	0		
Input		59	25.0	1.00	l	6000	6000											
		60	25.0	1.00	l	6000	6000											
Waste		61	26.6	1.00	l	-6018	-6000	0	0	0	0	-17.8	-0.140	0	0	0	0	0
		62	26.6	1.00	s	1834	833	100.0	0	899	0	2.47	0.0195	0	0	0		

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Water	Palladium	palladium chloride	activated carbon	Pd(OH)4 on C	Formaldehyde	Carbon dioxide	Sodium hydroxide	Hydrogen peroxide	Sodium chloride	Steam	Water
		63	100	1.00	g	834	832					2.47						
Waste		64	25.0	1.00	l	-834	-832	0	0	0	0	-2.47	0	0	0	0	0	0
		65	100	1.00	s	1000	1.00	100.0	0	899	0	0	0.0195	0	0	0		
Main product		66	25.0	1.00	s	-1000	-1.00	-100.0	0	-899	0	0	-0.0195	0	0	0	0	0
		Product purity (%)				99.9												
		Main product				Palladium												
		Overall Rxn coefficients					3.00		-1.00			-1.00	1.00	-2.00	-1.00	2.00		
		Total yield of process (from reactant)					NA	NA	99.0			10.0	NA	33.6	94.3	NA		
Waste		Fugitive Losses (Total)			g	-1.61	0	0	0	0	0	-1.41	-0.197	0	0	0	0	0
		Input Sum				6.92E+04	6.75E+04	0	168	900	0	282	0	224	33.9	117		
		Fugitive Replacement of Reactants				1.41			0			1.41		0	0			
		Total Input (Input + Fugitive Replacement)				6.92E+04	6.75E+04	0	168	900	0	284	0	224	33.9	117		
		Product Sum				1000	1.00	100.0	0	899	0	0	0.0195	0	0	0		
		Main product flow				1000	1.00	100.0	0	899	0	0	0.0195	0	0	0		
		Net Input (in - out, omitting fugitives)				0.154												
Input		C1	20.0	1.00	l	0												
Input		C1	20.0	1.00	l	2252												2252
Cooling out		C2	50.0	1.00	l	2252	0	0	0	0	0	0	0	0	0	0	0	2252
Input		C3	20.0	1.00	l	1.57E+04												1.57E+04
Cooling out		C4	50.0	1.00	l	1.57E+04	0	0	0	0	0	0	0	0	0	0	0	1.57E+04
Input		C5	20.0	1.00	l	5.00E+04												5.00E+04
Cooling out		C6	50.0	1.00	l	5.00E+04	0	0	0	0	0	0	0	0	0	0	0	5.00E+04
Input		C7	20.0	1.00	l	692												692
Cooling out		C8	50.0	1.00	l	692	0	0	0	0	0	0	0	0	0	0	0	692
Input		C9	20.0	1.00	l	752												752
Cooling out		C10	50.0	1.00	l	752	0	0	0	0	0	0	0	0	0	0	0	752
Input		C11	20.0	1.00	l	990												990
Cooling out		C12	50.0	1.00	l	990	0	0	0	0	0	0	0	0	0	0	0	990
Input		C13	20.0	1.00	l	1.43E+04												1.43E+04

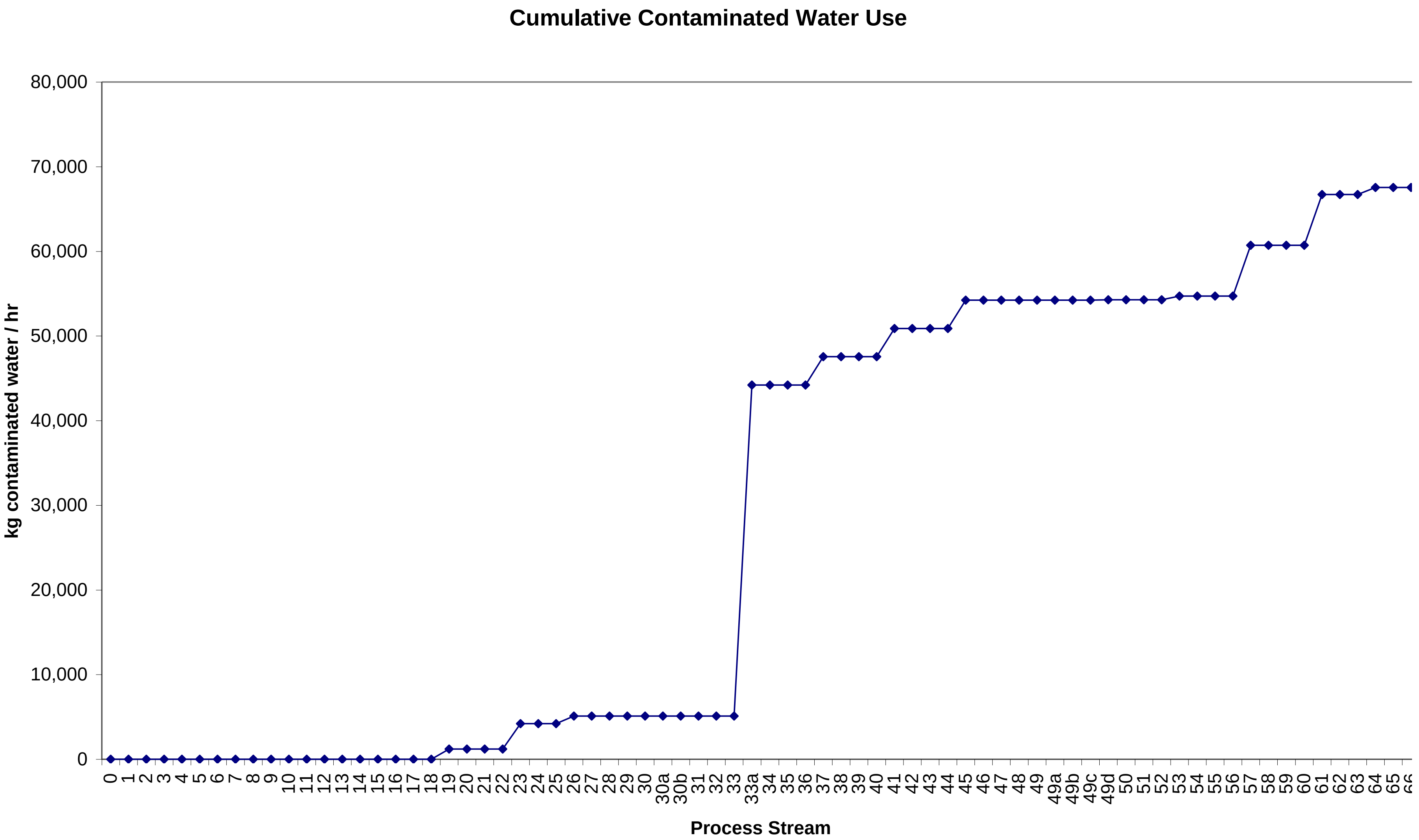
	Comments	Streams	Temp [C]	P	Phase	Total Flow	Water	Palladium	palladium chloride	activated carbon	Pd(OH)4 on C	Formaldehyde	Carbon dioxide	Sodium hydroxide	Hydrogen peroxide	Sodium chloride	Steam	Water
Cooling out		C14	50.0	1.00	l	1.43E+04	0	0	0	0	0	0	0	0	0	0	0	1.43E+04
Input		C15	20.0	1.00	l	395												395
Cooling out		C16	50.0	1.00	l	395	0	0	0	0	0	0	0	0	0	0	0	395
Input		S1	207	1.00	l	388											388	
Steam out		S2	207	1.00	l	388	0	0	0	0	0	0	0	0	0	0	388	0
Input		S3	207	1.00	l	1413											1413	
Steam out		S4	207	1.00	l	1413	0	0	0	0	0	0	0	0	0	0	1413	0
Input		S5	207	1.00	l	4553											4553	
Steam out		S6	207	1.00	l	4553	0	0	0	0	0	0	0	0	0	0	4553	0
Input		C1	20.0	1.00	l	2252												2252
Cooling out		C2	50.0	1.00	l	-2252	0	0	0	0	0	0	0	0	0	0	0	-2252
Input		C3	20.0	1.00	l	1.57E+04												1.57E+04
Cooling out		C4	50.0	1.00	l	-1.57E+04	0	0	0	0	0	0	0	0	0	0	0	-1.57E+04
Input		C5	20.0	1.00	l	5.00E+04												5.00E+04
Cooling out		C6	50.0	1.00	l	-5.00E+04	0	0	0	0	0	0	0	0	0	0	0	-5.00E+04
Input		C9	20.0	1.00	l	752												752
Cooling out		C10	50.0	1.00	l	-752	0	0	0	0	0	0	0	0	0	0	0	-752
Input		C11	20.0	1.00	l	990												990
Cooling out		C12	50.0	1.00	l	-990	0	0	0	0	0	0	0	0	0	0	0	-990
Input		C13	20.0	1.00	l	1.43E+04												1.43E+04
Cooling out		C14	50.0	1.00	l	-1.43E+04	0	0	0	0	0	0	0	0	0	0	0	-1.43E+04
Input		C15	20.0	1.00	l	395												395
Cooling out		C16	50.0	1.00	l	-395	0	0	0	0	0	0	0	0	0	0	0	-395
Input		S1	207	1.00	l	388											388	
Steam out		S2	207	1.00	l	-388	0	0	0	0	0	0	0	0	0	0	-388	0
Input		S3	207	1.00	l	1413											1413	

	Comments	Streams	Temp [C]	P	Phase	Total Flow	Water	Palladium	palladium chloride	activated carbon	Pd(OH)4 on C	Formaldehyde	Carbon dioxide	Sodium hydroxide	Hydrogen peroxide	Sodium chloride	Steam	Water
Steam out		S4	207	1.00	l	-1413	0	0	0	0	0	0	0	0	0	0	-1413	0
Input		S5	207	1.00	l	4315											4315	
Steam out		S6	207	1.00	l	-4315	0	0	0	0	0	0	0	0	0	0	-4315	0
Input		S7	207	1.00	l	126											126	
Steam out		S8	207	1.00	l	-126	0	0	0	0	0	0	0	0	0	0	-126	0
Input		S9	207	1.00	l	1331											1331	
Steam out		S10	207	1.00	l	-1331	0	0	0	0	0	0	0	0	0	0	-1331	0

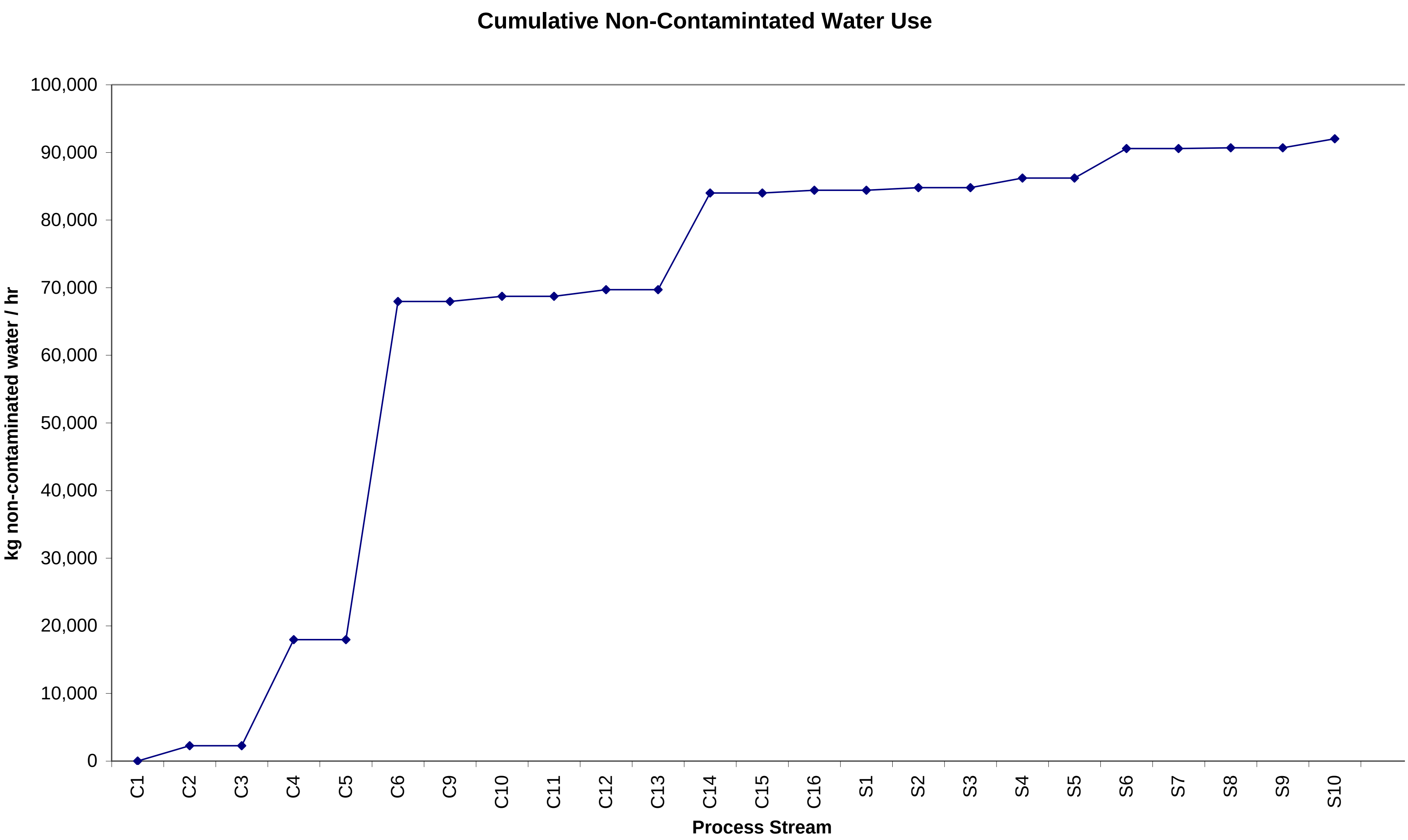
Graph of Cumulative Chemical Losses through Manufacturing Process



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 / batch]						Cooling Requirements [MJ / batch]							
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]
Cnv1	Conveyer 1	7.07E-04	7.07E-04		E	Hx2	Heat exchanger 2	-333	-333	90.0	0.250	-83.2	-83.2
P1	Pump 1	0.179	0.179		E	Hx3	Heat exchanger 3	-2319	-2651	120	0.250	-580	-663
Cnv2	Conveyer 2	4.90E-04	0.180		E	Hx4	Heat exchanger 4	-7383	-1.00E+04	70.0	0.250	-1846	-2509
MxEl1	Mixing electricity 1	4.81	4.99	0	E	Hx5	Heat exchanger 5	-111	-1.01E+04	100	0.250	-27.7	-2536
P2	Pump 2	0.0428	5.03		E	Hx6	Heat exchanger 6	-146	-1.03E+04	100	0.250	-36.5	-2573
Cnv3	Conveyer 3	3.78E-03	5.04		E	Hx7	Heat exchanger 7	-2111	-1.24E+04	100	0.250	-528	-3101
Hx1	Heat exchanger 1	631	636	90.0	S	Hx8	Heat exchanger 8	-58.3	-1.25E+04	100	0.250	-14.6	-3115
MxEl2	Mixing electricity 2	2.91	639	0	E								
P3	Pump 3	0.462	639		E								
P4	Pump 4	0.0735	639		E								
Dry1	Dryer 1	2297	2936	120	S								
P6	Pump 6	0.501	2937		E								
P7	Pump 7	1.00E-05	2937		E								
R1	Reactor 1	7013	9.95E+03	70.0	S								
MxEl2	Mixing electricity 2	18.6	9.97E+03	0	E								
P8	Pump 8	3.62	9.97E+03		E								
P9	Pump 9	8.47E-03	9.97E+03		E								
P10	Pump 10	8.47E-03	9.97E+03		E								
P11	Pump 11	8.47E-03	9.97E+03		E								
P11a	Pump 11a	7.40E-04	9.97E+03		E								
R2	Reactor 2	205	1.02E+04	100	S								
P12	Pump 12	0.150	1.02E+04		E								
P13	Pump 13	0.0427	1.02E+04		E								
P14	Pump 14	0.0427	1.02E+04		E								
Dry2	Dryer 2	2164	1.23E+04	100	S								
	Potential recovery	-3115	9225										
	Net energy		9225				Potential recovery:						-3115

	Electricity	31.4	E	[MJ/hr]									
	DowTherm	0	D	[MJ/hr]									
	Heating steam	1.23E+04	S	[MJ/hr]									
	Direct fuel use	0	F	[MJ/hr]									
	Heating natural gas	0	G	[MJ/hr]									
	Energy input requirement	1.23E+04		[MJ/hr]									
	Cooling water	-1.25E+04		[MJ/hr]									
	Cooling refrigeration			[MJ/hr]									
	Potential heat recovery	-3115		[MJ/hr]									
	Net energy	9225		[MJ/hr]									

Graph of Cumulative Energy Requirements