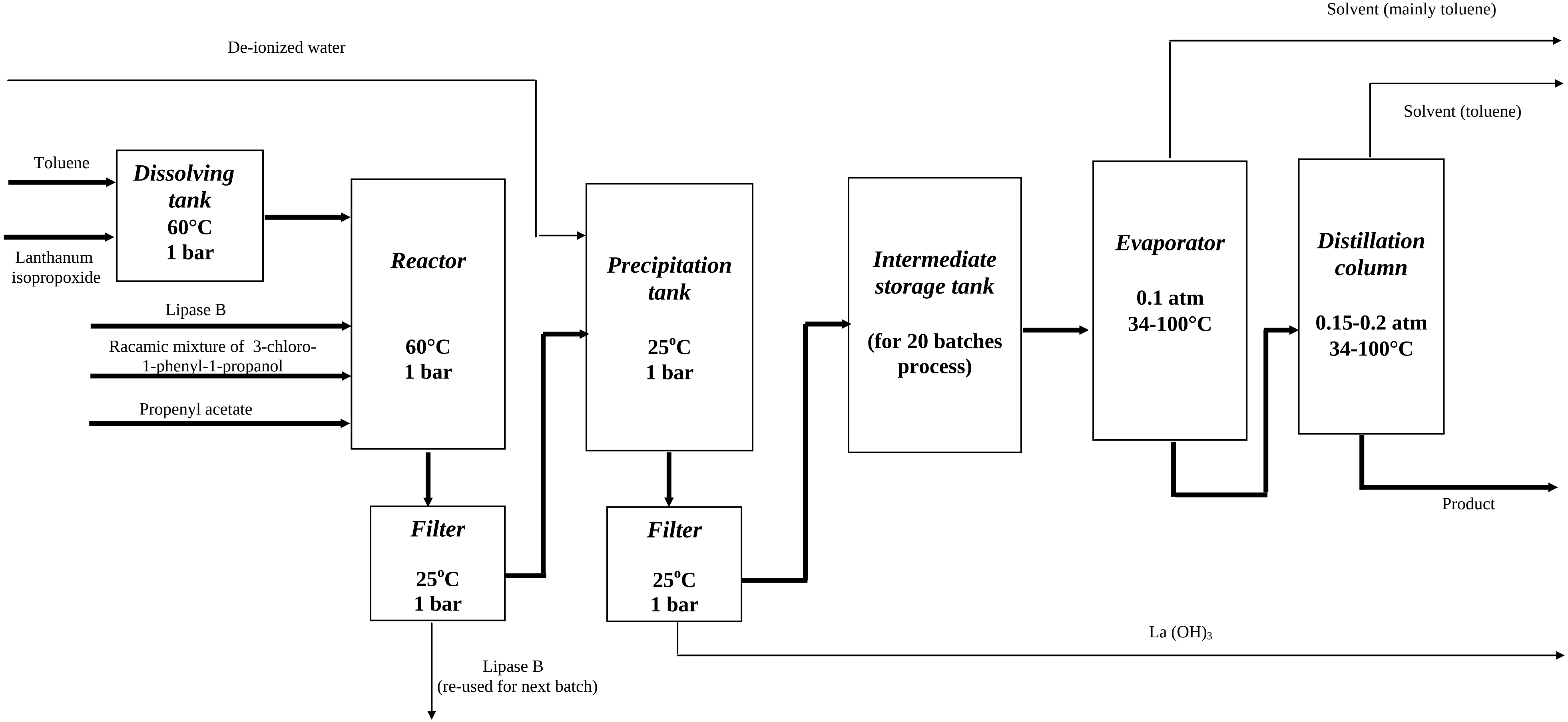
APPENDICES

APPENDIX A1 PROCESS OPTIONS

A1.1 Block schemes of the process options

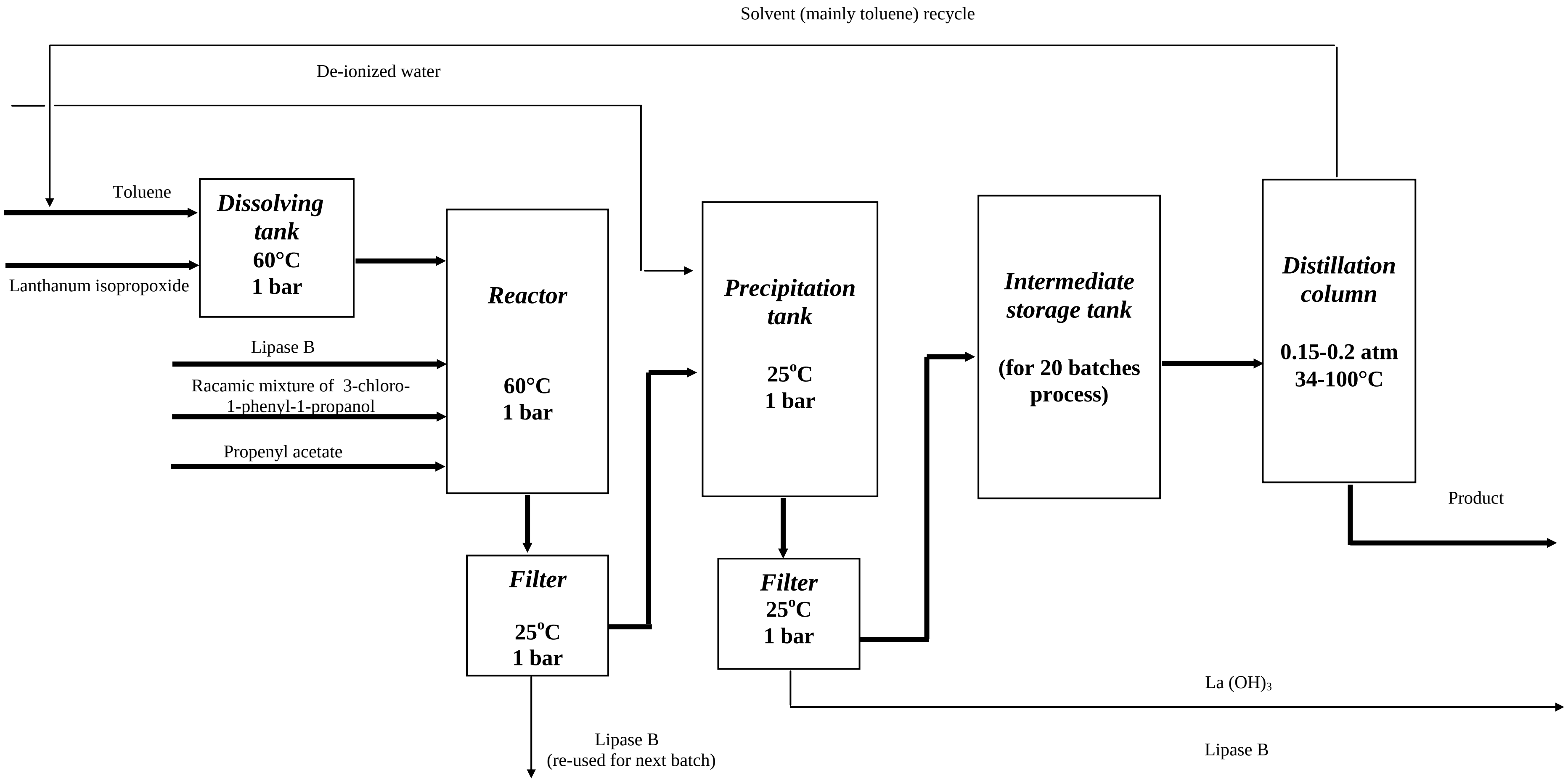
Option 1

Figure A1.1.1 Block scheme of process option 1 to the precursor of Prozac (3-chloro-1-phenyl propyl acetate)



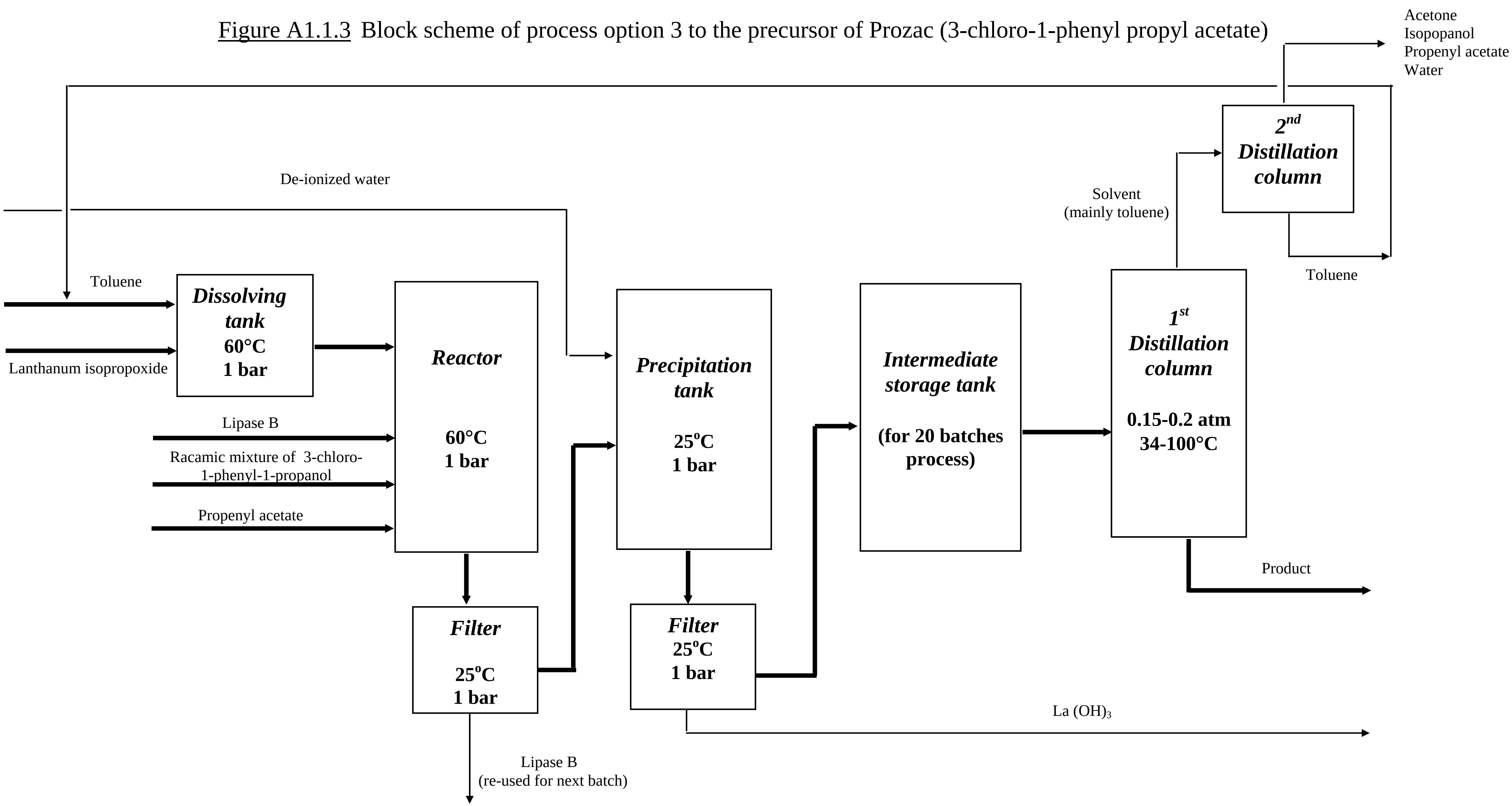
Option 2

Figure A1.1.2 Block scheme of process option 2 to the precursor of Prozac (3-chloro-1-phenyl propyl acetate)



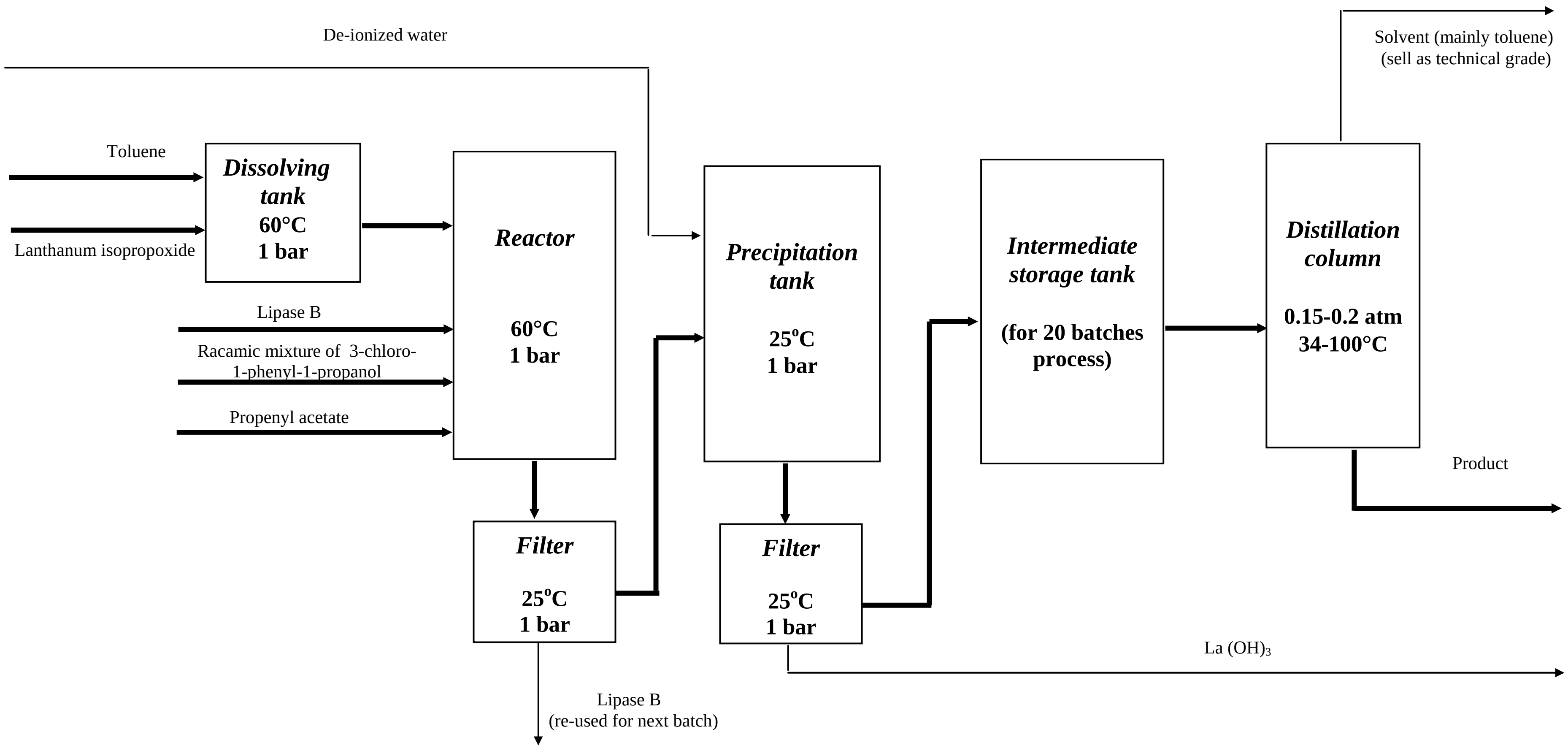
Option 3

Figure A1.1.3 Block scheme of process option 3 to the precursor of Prozac (3-chloro-1-phenyl propyl acetate)



Option 4

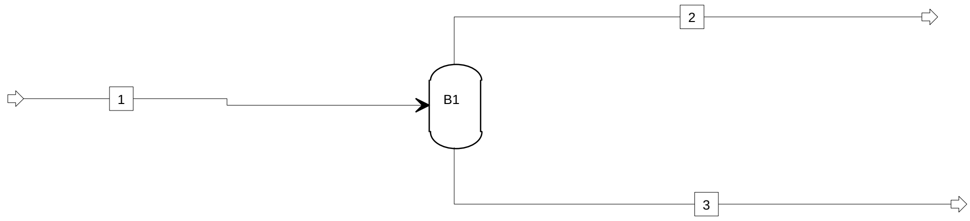
Figure A1.1.4 Block scheme of process option 4 to the precursor of Prozac (3-chloro-1-phenyl propyl acetate)



A1.2 The simulation (ASPEN PLUS model) for the option with the evaporator

If the evaporator is used to separate the toluene and precursor, it is necessary to check if the evaporator can separate these two substances effectively.

In Aspen, the flash model is used:



The stream 1 is the feed. The composition is the same as that in stream1 in appendix A5.10, table A5.10.1)
In block B1, the pressure is chosen as 0.15bar and temperature is chosen as 55°C. Then the simulation start and the results is shown in the table below:

Table A1.2.1: The simulation result using the evaporator for purification of product

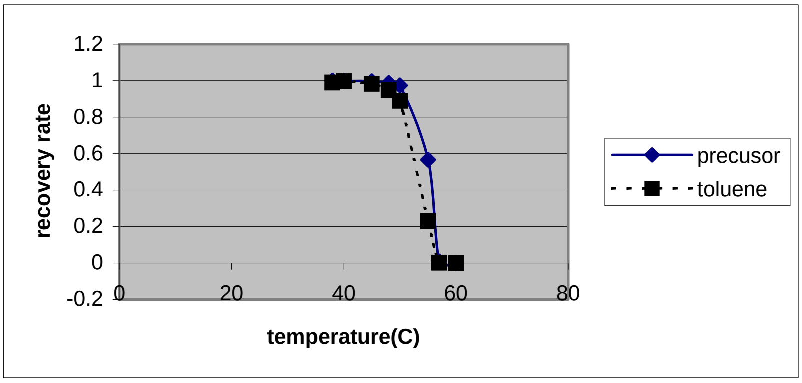
Mole Flow (kmol/sec)	Stream 1	Stream 2	Stream 3
PROPENEA	4.18E-05	3.62E-05	5.59E-06
PERCURSO	8.33E-05	3.62E-05	4.71E-05
REACTANT	1.05E-07	2.52E-10	1.05E-07
ACETO-01	8.33E-05	8.02E-05	3.09E-06
TOLUE-01	0.00196	0.001508	0.000452
WATER	9.39E-06	9.37E-06	1.68E-08
ISOPR-01	1.88E-05	1.83E-05	4.75E-07

Recover rate of precursor (in stream 3) is 4.71E-05/8.33E-05 = 0.566
Recover rate of toluene (in stream 3) is 4.52E-04/1.96E-03 = 0.23

The result shows that 43% precursor is lost in the vapor stream 2 when 77% toluene is separated from the precursor. It is not good because too much precursor is lost.

Varying the temperature from 38°C to 60°C, simulate again and the result is shown in the following graph:

Figure A1.2.1: The recovery rate vs the temperature chosen for the evaporator



From the graph, the following conclusion is drawn:

1) In low temperature range (<50°C), toluene cannot be separated from the precursor effectively. Most toluene will go with precursor in the product stream 3.
2) In medium temperature range (50~57°C), some toluene can be separated from the precursor, but in the same time the loss of precursor is high.
3) In high temperature range (>57°C), toluene cannot be separated from the precursor effectively. Most toluene will go with precursor in the vapor stream 1.

When the pressure is varied, the similar conclusion can be drawn as the above.

So, from the simulation results in Aspen, it is not good to separate toluene from precursor by evaporator because the loss of the product (the precursor of Prozac) is high via separation.

APPENDIX A2 ESTIMATION OF MARGIN AND MAXIMUM ALLOWED INVESTMENT

A2.1 Estimation of margin

Table A2.1: Estimation of margin

Component	***Stream number***	***Density*** *kg/L*	*Dfl/L*	***Price*** *Dfl/kg*	*Dfl/t*	***IN*** *kg/year*	*t/a*	***Value*** *Dfl/year*	*Euro/year*
Feed stock									
Lipase B from *Candida Antarttica* (4)	<1>			30,000.00	30,000,000.00	8.80	0.009	264,000.00	120,000.00
Lanthanum isopropoxide (2)	<2>			48,333.00	48,333,000.00	569.70	0.570	27,535,310.10	12,516,050.05
Toluene	<3>	0.87	12.88	14.80	14,804.60	52,012.00	52.012	770,016.74	350,007.61
(R&S)-3 chloro 1-phenyl-1-propanol (3)	<5>			500.00	500,000.00	4,096.00	4.096	2,048,000.00	930,909.09
Propenyl acetate (1)	<6>			47.70	47,700.00	3,608.00	3.608	172,101.60	78,228.00
Deionized water (5)	<8>	1.00	40.00	40.00	40,000.00	145.94	0.146	5,837.60	2,653.45
Total raw materials cost								**30,795,266.04**	**13,997,848.20**
Product						**OUT**			
Precursor of Prozac	<14>			10,000.00	10,000,000.00	5,095.00	5.095	50,950,000.00	23,159,090.91
R-3chloro 1-phenylpropyl acetate (6)									
Total product value								**50,950,000.00**	**23,159,090.91**
By products									
Lanthanum hydroxide (7)	<10>			500.00	500,000.00	342.00	0.342	171,000.00	77,727.27
Technical grade toluene (8)	<13>			3.00	3,000.00	54,990.00	54.990	164,970.00	74,986.36
Total by-products value								**335,970.00**	**152,713.64**
MARGIN (= product value + by-products value – raw materials cost)								**20,490,703.96**	**9,313,956.35**

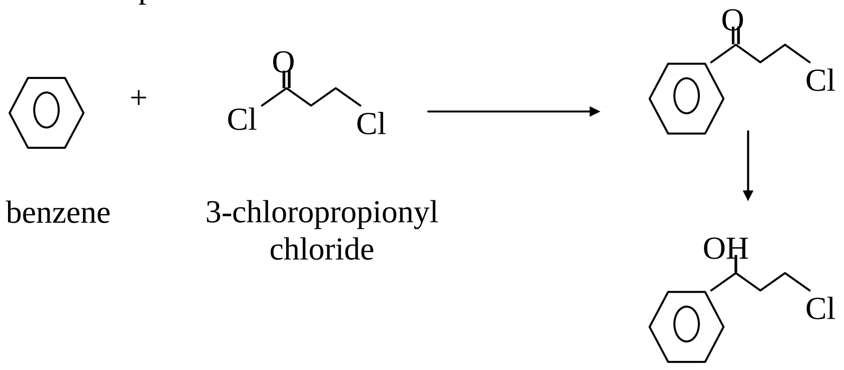
Remarks:

(1) The price of enzyme is estimated based on the price of 4000Dfl/100g (given by the Principal [6]). The price of 3000Dfl/100g is estimated for purchasing of large quantity (refer to part 2.3, chapter 2 for the amount of lipase B needed)

(2) The price of catalyst Lanthanum isopropoxide is estimated based on the price by Alfa Chemicals, which is 725Dfl/10g or 72,500Dfl/kg. Since this price is for purchasing small quantity. The price for purchasing large quantity is estimated to be 2/3 of the above price.

(3) The price of toluene is from Acros Organics

(4) The price of racemic mixture of 3-chloro-1-phenyl -1-propanol is estimated from the price of benzene and 3-chloro propionyl chloride
Since the material is not commercially available, its price is estimated based on benzene and 3-chloropropionyl chloride. This material can be produced from these 2 compounds



(R-, S-) 3-chloro-1-phenyl-1-propanol

	benzene +	3-chloropropionyl chloride	⟶	3 chloro-1 phenyl-1propanol
	1 kmol	1 kmol		1 kmol
	78.11kg	126.97 kg		170.5kg
	0.458kg	0.745kg	⟶	1kg
Price (Dfl/kg)	12.11	462.1		
Cost (Dfl	5.546	344.26	Price	349.81

(the prices for benzene and 3-chloropropionyl chloride are from Across Organics)

However, it is not realistic if it is assumed to be 100% conversion for the above reaction so the price for 3 chloro-1- phenyl-1-propanol should be higher than the above estimated price. In addition, the processing cost should be taken into consideration.

Therefore, the price for 3 chloro-1- phenyl-1-propanol is estimated to be 500 Dfl/kg

(5) The price of propenyl acetate is estimated based on the price of isopropenyl acetate by Acros Organics.

(6) The price of de-ionized water is estimated based on the price offered by Alfa Chemicals. They sell at about 45Dlf /L for purchasing of small quantity.

(7) The price of the product (precursor of Prozac) is estimated based on the price of (R)-3-chloro-1-phenyl-1-propanol because this precursor is not commercially available. (R)-3-chloro-1-phenyl-1-propanol is chosen for the estimation of the price because it is also pure enantiomer and the chemical structure has a lot of similarities to the product. The price of (R)-3-chloro-1-phenyl-1-propanol is estimated from the price by Sigma-Aldrich. They sell this product at the price 217.5DM/5g i.e about 45,000Dfl/kg for a small quantity. The price of the product (precursor of Prozac) is estimated to be approximately 20% of this price (for large quantity purchasing)

(8) The price of technical grade toluene (95% wt toluene) is estimated to be 3Dfl/kg after consult with some colleagues. The normal price in the world market for technical grade toluene (70% wt toluene) is in the range 0.25-0.5 USD/kg (i.e 0.6-1.25 Dfl/kg).

(9) The price to sell Lanthanum hydroxide is estimated based on the price of Alfa Chemicals. They sell this product at a price of almost 800Dfl/kg for purchasing small quantity

A2.2 Determination of maximum acceptable investment at DCFROR of 10%

$$\text{Present margin} = \frac{\text{Margin}}{(1+r)^n}$$

$$\text{Cumulative of margin in working years} = \sum_{n=2}^{n=11} \frac{\text{Margin}}{(1+r)^n}$$

$$\text{DCFROR} = \frac{\text{Cumulative net cash flow at the end of project}}{\text{Life of project} \times \text{Original investment}}$$

$$\text{DCFROR} = \frac{\text{Cumulative of margin in working years - Original investment}}{\text{Life of project} \times \text{Original investment}}$$

As DCFROR is 10% or 0.1:

$$\frac{\text{Cumulative of margin in working years - Original investment}}{\text{Life of project} \times \text{Original investment}} = 0.1$$

$$\rightarrow \text{Original investment} = \frac{\text{Cumulative of margin in working years}}{0.1\times \text{Life of project} + 1}$$

Year	*Present margin*
2	17,567,476.00
3	16,266,181.00
4	15,061,279.00
5	13,945,629.00
6	12,912,619.00
7	11,956,129.00
8	11,070,490.00
9	10,250,453.00
10	9,491,160.60
11	8,788,111.70

Cumulative for margin in working years	
127,309,529.00	Dfl
Original Investment	
60,623,585.00	Dfl

When DCFROR (Discount Cash Flow rate of Return) is 10% the maximum acceptable investment is 60,623,585.00 Dfl.

APPENDIX A3 PROCESS STRUCTURE AND DESCRIPTION

A3.1 Nitrogen injection

A3.1.1 The amount of nitrogen injected

Nitrogen is injected into the dissolving tank T102 and the reactor R101 to “push” out the air inside these unit operations. It is essential to have dry conditions inside the dissolving tank and the reactor because lanthanum isopropoxide is very sensitive to water.

It is designed to inject the nitrogen into these unit operations 2 times: before adding the raw materials and after. It is necessary to inject nitrogen after adding raw materials into these unit operations because air might get into the tank and the reactor when raw materials are added.

The amount of nitrogen injected before adding raw materials is equivalent to 1.5 times of the volume of these equipments. This is an assumption to make sure that sufficient amount of nitrogen injected to obtain dry condition.

The dissolving tank and reactor is designed so that the reaction mixture occupies only 75% of the total volume. Therefore, there is 25% of total volume is empty “headspace”. The amount of nitrogen injected after adding raw materials is equivalent to 2 times of the volume of the “headspace”, which is 50% (or 0.5 times)of the volume of dissolving tank and the reactor. It is again an assumption to ensure that dry condition is achieved inside these equipments.

Table A3.1 The amount of nitrogen injected

Equipment	*Volume (m^3)*	*1^{st} injection ($\times$1.5 V) (m^3/batch)*	*2^{nd} injection ($\times$0.5V) (m^3/batch)*	*Total amount injected (m^3/batch)*	*Number of batches*	*Total amount injected (m^3/a)*
T102 Dissolving tank	0.75	1.13	0.38	1.51	100	151.0
R101 Reactor	0.83	1.25	0.42	1.68	100	168.0
Total						**319.0**
Remarks: - refer to appendix A5.2 and A5.3 for dissolving tank T102 and reactor R101 design						

A3.1.2 Determination of the time needed for each injection

Calculation of the flow rate of nitrogen

Velocity v = 20 m/s (assumption for gas)
Diameter of the pipe: D = 1cm = 10^{-2} m
Area of the pipe A = $(\pi/4)\times D^2 = (\pi/4)\times (10^{-2})^2$ m^2

Flow rate F = $v \times A = 20 \times (\pi/4) \times (10^{-2})^{2} = 0.00157$ m^3/s = 5.652 m^3/h

Injected time $t_{injected}\left(\min\right) = \dfrac{V_{injected}\left(m^3\right)}{Flow\ rate\left(\dfrac{m^3}{h}\right)} \times 60\left(\dfrac{\min}{h}\right)$

Table A3.2 The time needed for each injection

Equipment	*1st injection ($\times$1.5 V) (m^3/batch)*	$t_{injected}$ *(min)*	*2nd injection ($\times$0.5V) (m^3/batch)*	$t_{injected}$ *(min*
T102 Dissolving tank	1.13	12.0	0.38	4.0
R101 Reactor	1.25	13.3	0.42	4.5

A3.2 Utilities summary

SUMMARY OF UTILITIES																
EQUIPMENT		**UTILITIES**														
		Heating					**Cooling**				**Power**				**Dry**	***Remarks***
Nr.	**Name**	Load	Consumption (t/a)				Load	Consumption (t/a)			Actual	Consumption (t/a, kWh/a)			Consumption	
			Steam			Hot		Cooling	Air	Refrig.	Load	Steam (t/h)		Electricity	Nitrogen	
		kW	LP	MP	HP	Oil	kW	Water			kW	HP	MP	kWh/a	(m^3)	
T102	Dissolving tank														150,8	refer to appendix 3.1
R101	Reactor														168,0	
T102	T102 stirrer										0,2			1,3		refer to appendix A5.2 of T102 design
R101	R101 stirrer										0,2			88,8		refer to appendix A5.3 for reactor R101 design
R101	R101 heating	45,5	1,6													refer to appendix A4.3
R101	R101 during reaction						0,7	7,1								refer to part 5.5 for reason of chosing CW
R101	R101 Cooling down						10,3	69,7								
F101	F101 drive force													666,7		
T103	T103 Stirrer										0,2			2,8		refer to appendix A5.5 fro precipitation tank design
F102	F102 drive force										16,0			666,7		Superpro- default data
E101	C101 feed heat.	25,2	3,3													refer to appendix A4.3.
E103	C101 Reboiler	100,2	13,4													refer to part 5.5 for reason of chosing LP steam
E102	C101 Cond.						121,0	833,8								
P101	T102 Feed										1,5			25,0		refer to equipment sheets for pumps in chapter 8
P102	R101 Feed										1,3			10,8		
P103	T103 Feed										0,7			23,3		
P104	C101 feed										0,7			56,0		
P106	C101 Reflux										0,1			8,0		
P107	C101 Product										0,5			36,0		
P108	C101 Bottoms										0,0			0,8		
P105	C101 Vacumm pump										2,8			224,0		
E104	Product cool						1,6	10,7								
TOTAL			**18,24**					**921,4**						**1810,1**	**318,8**	

Project ID Number :	**CPD** 3265	
Completion date :	21 Dec 2001	

APPENDIX A4 MASS AND HEAT BALANCE

A4.1 Batch remarks and calculation

Table A4.1 Batch remarks and calculations

Calculations :

Dimensions

Quantity	Unit
Time	h or annum
Mass	kg or t
Flow	kg/h
Energy	MJ
Power	kW
Pressure	bar
Temp	C

Input data and derived values

Production	
(R)-3-chloro-1-phenylpropyl acetate	5100 [kg/a]
Toluene	55 [t/a]
Lanthanum Hydroxide	342 [kg/a]
h_{str}	100 [days/a]

Main Reaction (weight basis)
2.936 A + 1.724 B ---> 3.659 C + D
Exothermic reaction requires cooling
Conversion reactants A : 99.9 %
Feed A:B = 1 : 0.881 (weight basis)
Note : A,B,C,D are given above

Precipitation reaction (weight basis)
5.855 E + F --> 3.5172 G + 3.338 H
Conversion reactants E : 100%
Note: E,F,G,H are given above

Energy and Power

Component	Symbol	Enthalpy (H) [kJ/kg] 20° C	30° C	60° C
Toluene		123.776	140.373	193.140
R-, S- 3-chloro-1-phenyl-1-propanol	A	-1736.757	-1725.187	-1687.126
Propenyl Acetate	B	-3872.187	-3854.096	-3797.432
(R)-3-chloro-1-phenylpropyl acetate	C	-2058.905	-2048.301	-2014.203
Isopropanol	H	-5294.513	-5265.853	-5175.293
Acetone	D	-4262.929	-4241.852	-4175.966
Lanthanum Isopropoxide (solid)		-6.087	6.087	42.607
Water	F	-15877.060	-15838.580	-
Lanthanum Hydroxide (solid)	G	-2.943	2.943	20.602
Lanthanum Isopropoxide (liquid)	E	-116.143	-114.213	-108.013

Calculation of energy and power

Parameter	Unit	Factor
Flow	kg/h	
mass per batch	kg	
H	kJ/kg	
H * mass per batch	kJ	
H * Flow/Factor	kW	3600

Cycle times		Unit	Remarks
t 1st nitrogen injection	12.0	[min]	
t feed toluene to T102	10.0	[min]	
t feed La-Isopropoxide to T102	10.0	[min]	
t 2nd nitrogen injection to T102	4.0	[min]	
t dissolving in T102	10.0	[min]	
t discharge from T102 and feed to R101	5.0	[min]	
t feed racemic to R101	15.0	[min]	
t propenyl acetate	15.0	[min]	
t feed lipase B to R101	10.0	[min]	
t 2nd nitrogen injection to R101	4.5	[min]	
t heating	12.7	[min]	
t reaction and cooling	257.3	[min]	= t_{reac} = 4.5h = 270min
t cooling down	47.0	[min]	
t filtration in F101	25.0	[min]	- t total for these 3 steps is 30 mins (refer to table 5.1 for explanation
t feed to T103	20.0	[min]	
t feed water to T103	5.0	[min]	- feeding water while feed liquid to T103
t precipitation in T103	10.0	[min]	
t filtration	25.0	[min]	
t idle	962.5	[min]	
t total	24.0	[h]	= t_{batch}

Parameter	Description	Value	Unit	Calculation	Remarks
T feed	all feeds go to reactor	20	°C	Assumed	The process is inside building and some feeds are in liquid form
T heating up	Temp heating up	60	°C	Given	The feeds need to be heated until the desired reaction temperature
T react&cooling	Temp of reaction	60	°C	Given	The reaction goes well in 60°C (in consultation with Dr. Ulf Hanefeld)
T cooling down	Temp.end Cooling Down	30	°C	Assumed	* Cooling temperature of the reaction mixture to acceptable room temperature * If the temperature is lower than 30°C, it will need more time to cool and more cooling water rate * If the temperature is higher than 30°C, it's (a bit) too high for normal room temperature * 30°C is acceptable and also safe for workers near by (if any)
T water	Temp.of feed water	20	°C	Assumed	The feed water is at (inside) room temperature (20C)
T precipitation	Temp.of precipitation	30	°C	Assumed	The temperature will not change very much because: * the amount of reacted catalyst is very small (5.697 kg/batch) compared to the whole mixture (602.848 kg/batch) * the structure of reactant and product doesn't very much different therefore it won't make any difference in heat * the precipitation reaction is very fast (one droplet of water can precipitate the catalyst) * reaction condition is non-adiabatic
T filtration	Temp.of filtration	30	°C	Assumed	The temperature will not change throughout the pipe
T dis	Temp.of feed to dist.clm	88	°C	Given	From ASPEN, please refer to appendix A4.3.2
T top	Temp.of top product	34	°C	Given	From ASPEN, please refer to Apendix A4.3.2
T bottom	Temp.of bottom product	100	°C	Given	From ASPEN, please refer to Apendix A4.3.2
P column	Pressure in the column	0.15	atm	Given	From ASPEN, please refer to Apendix A4.3.2
t total	total cycle time	24	h	Calculated	= t_{batch}
n	Batch cycle per annum	100	[-]	h_{str} / t_{batch}	
Pr	Production rate	5000	kg/a	Given	
F	Correction factor	2%	[-]	Assumed	assumed that 2% of liquid flow will attach along pipes during the process
P actual	Actual production rate	5100	kg/a	Pr *F	
C batch	Product C / batch	51	kg	P actual/ h str	
A batch	Reactant A / batch	40.96	kg	Stoichiometry	See stoichiometry equation of main reaction
Fr	Ratio of A and B in feed	0.88	[-]	Given	See table "main reaction (weight basis)"
B batch	Reactant B / batch	36.08	kg	A batch*Fr	
D batch	Product D / batch	13.94	kg	Stoichiometry	
La-prop batch	Lanthanum Isoprop / batch	5.697	kg	Given	
Lipase batch	Lipase B / batch	8.8	kg	Given	Lipase B catalyst will stay in the reactor and the activity will be checked
Toluene batch	Toluene / batch	520.12	kg	Given	
F water	Excess water factor	50%	[-]	Assumed	Excess water is needed to make sure that the precipitation reaction occurs
De-ionized water	De-ionized water feed / batch	1.46	kg	Stoic.&Excess	See stoichiometry equation of precipitation
P $La(OH)_3$	$La(OH)_3$ produced / batch	3.422	kg	Stoichiometry	
P Isopropanol	Isopropanol produced / batch	3.25	kg	Stoichiometry	

Notes:

For calculation in the distillation column please refer to Appendix A.5.7

The calculation in the distillation column is done with ASPEN PLUS SIMULATION engine

A4.2 Process stream summary of separation part

Table A.4.2.1: Process stream summary of separation part

Stream Nr.		<22>		<23>		<24>		<25>	
Name		to E101	IN	to C101		to E102		to V103	
Component	Mwt	Flow		Flow		Flow		Flow	
		kg/h	kmol/h	kg/h	kmol/h	kg/h	kmol/h	kg/h	kmol/h
Toluene	92.14	650.141	7.056	650.141	7.056	942.570	10.230	942.570	10.230
La-Isopropoxide	316.18	-	-	-	-	-	-	-	-
R-, S- 3-chloro-1-phenyl-1-propanol	170.5	0.064	0.000	0.064	0.000	0.000	0.000	0.000	0.000
Lipase B		-	-	-	-	-	-	-	-
Propenyl Acetate	100.12	15.063	0.150	15.063	0.150	21.841	0.218	21.841	0.218
(R)-3-chloro-1-phenylpropyl acetate	212.5	63.750	0.300	63.750	0.300	0.309	0.001	0.309	0.001
Acetone	58.08	17.424	0.300	17.424	0.300	25.265	0.435	25.265	0.435
Water	18	0.609	0.034	0.609	0.034	0.883	0.049	0.883	0.049
Lanthanum Hydroxide	189.9	-	-	-	-	-	-		-
Isopropanol	60.1	4.062	0.068	4.062	0.068	5.890	0.098	5.890	0.098
Total		751.104	7.908	751.104	7.908	996.758	11.031	996.758	11.031
Enthalpy : kW		-59.719		-34.518		93.977		-27.045	
Phase		L		L		V		L	
Pressure : bar		5.2		1		0.15		0.15	
Temperature : C		20		88.1		53.7		34	

Table A.4.2.1: Process stream summary of separation part (cont'd)

Stream Nr.		<26>		<27>		<28>		<29>	
Name		to P106		to C101		to P107		to T105	OUT
Component	Mwt	Flow		Flow		Flow		Flow	
		kg/h	kmol/h	kg/h	kmol/h	kg/h	kmol/h	kg/h	kmol/h
Toluene	92.14	292.522	3.175	292.522	3.175	650.048	7.055	650.048	7.055
La-Isopropoxide	316.18	-	-	-	-	-	-	-	-
R-, S- 3-chloro-1-phenyl-1-propanol	170.5	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Lipase B		-	-	-	-	-	-	-	-
Propenyl Acetate	100.12	6.778	0.068	6.778	0.068	15.063	0.150	15.063	0.150
(R)-3-chloro-1-phenylpropyl acetate	212.5	0.096	0.000	0.096	0.000	0.213	0.001	0.213	0.001
Acetone	58.08	7.841	0.135	7.841	0.135	17.424	0.300	17.424	0.300
Water	18	0.274	0.015	0.274	0.015	0.609	0.034	0.609	0.034
Lanthanum Hydroxide	189.9	-	-	-	-	-	-	-	-
Isopropanol	60.1	1.828	0.030	1.828	0.030	4.062	0.068	4.062	0.068
Total		309.339	3.424	309.339	3.424	687.381	7.608	687.381	7.608
Enthalpy : kW		-8.393		-8.393		-18.652		-18.652	
Phase		L		L		L		L	
Pressure : bar		0.15		1.7		0.14		4	
Temperature : C		34		34		34		34	

Table A.4.2.1: Process stream summary of separation part (cont'd)

Stream Nr.		<30>		<31>		<32>	
Name		to E104		to P108		to T106	OUT
Component	Mwt	Flow		Flow		Flow	
		kg/h	kmol/h	kg/h	kmol/h	kg/h	kmol/h
Toluene	92.14	0.093	0.001	0.093	0.001	0.093	0.001
La-Isopropoxide	316.18	-	-	-	-	-	-
R-, S- 3-chloro-1-phenyl-1-propanol	170.5	0.064	0.000	0.064	0.000	0.064	0.000
Lipase B		-	-	-	-	-	-
Propenyl Acetate	100.12	0.000	0.000	0.000	0.000	0.000	0.000
(R)-3-chloro-1-phenylpropyl acetate	212.5	63.537	0.299	63.537	0.299	63.537	0.299
Acetone	58.08	0.000	0.000	0.000	0.000	0.000	0.000
Water	18	0.000	0.000	0.000	0.000	0.000	0.000
Lanthanum Hydroxide	189.9	-	-	-	-	-	-
Isopropanol	60.1	0.000	0.000	0.000	0.000	0.000	0.000
Total		63.723	0.300	63.723	0.300	63.723	0.300
Enthalpy : kW		-34.686		-36.237		-36.237	
Phase		L		L		L	
Pressure : bar		0.15		0.6		3.7	
Temperature : C		34		25		25	

Mass and heat balance calculation steps:

1. Since the mass entering and going out from distillation column (stream <22>, <29>, <30>) is known, and the reflux ratio is also obtained from simulation (<27> / <25> = 0.45 / 1.45), then the other streams mass can be calculated from mass balance.

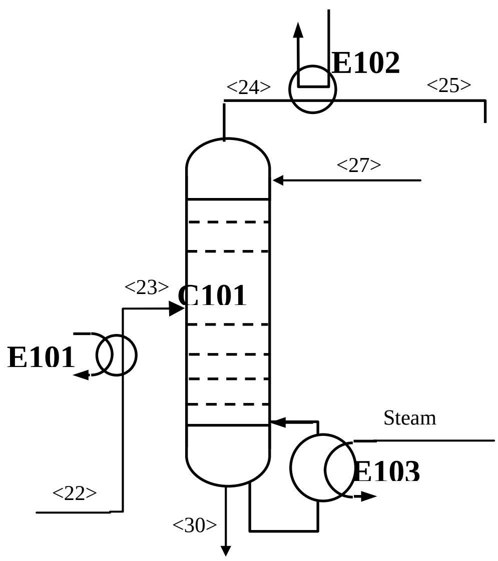


Figure A.4.2.1: Mass and heat balance boundary for distillation column C101

2. *Mass balance in C101:*
MASS IN = MASS OUT
<22> + <27> = <30> + <25>
751.104 + 0.45/1.45 × <25> = 63.723 + <25>
Hence, the mass in stream <25> is equal to 996.758 kg/h
From reflux ratio, the stream <27> = 0.45/1.45 × <25> = 309.339 kg/h

3. *Heat balance in C101:*
HEAT IN = HEAT OUT

- *Enthalpy of stream <22> + enthalpy of stream <27> + heat added to E101 + heat added to E103 = enthalpy of stream <25> + enthalpy of stream <30> + heat removed from E102.*

where:
- The enthalpy of stream <22>, <30>, and heat duty of each heat exchanger are known (please refer to table 5.2 for Process stream summary).
- From reflux ratio, the enthalpy of stream <27> = 0.45/1.45 × enthalpy of stream <25>.
- Applying the above heat balance, the enthalpy of stream <25> can be calculated, which is –27.045 kW.

→ The enthalpy of stream <27> is 0.45/1.45 × enthalpy of stream <25> = -8.393 kW

- *Heat balance in E102 can be made to calculate the enthalpy of stream <24>*

Enthalpy of stream <24> = enthalpy of stream <25> + heat removed from E102
= –27.045 + 121.023 = 93.977 kW.

- *The same heat balance can be made in E104 to calculate the enthalpy of stream <31>:*

Enthalpy of stream <31> = enthalpy of stream <30> - heat removed from E104:
= -34.686 – 1.551 = -36.237 kW.

A4.3 Design of heating and cooling system for the reactor R101 and distillation column C101

A4.3.1 Batch reactor R101

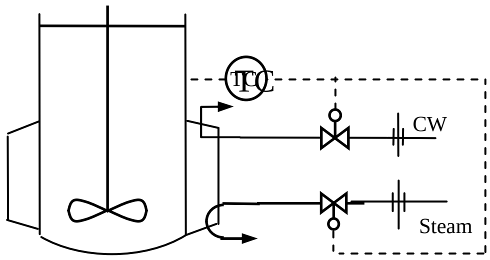
a) <u>*Kinetic assumptions*</u>*:*

- Total reaction time is 4.5 hours per batch (refer to part 2.4, chapter 2)
- Assumed it is an ideal batch reactor
- The reaction is first order reaction (Because the concentration of reactant is very low) (refer to part 2.4, chapter 2)
- Conversion is 99.9%

Hence: $t = C_{A0} \int_{0}^{0.999} \frac{d\xi}{kC_{A0}(1-\xi)}$ with t = 4.5h $\rightarrow$ k = 1.5351h^{-1}.

<u>Figure A4.1</u>: The batch reactor

R101



b) <u>*Heat balance when heating the reaction mixture (to 60^{o}C)*</u>

After all raw materials, whose initial temperature is 20^{0}C, are added into the reactor low-pressure steam, whose temperature is 110^{0}C and pressure is 1.5 bar, is used as hot utility to heat the reaction mixture to 60^{0}C.

Assume the reaction constant is the same at different temperatures, heat balance is written as:

Heat transferred + Heat produced = Temperature hold up

$$-UA(T_r - T_h) + (-\Delta H_{20\text{-}60C})(-R) = \rho V C_p \frac{dT_r}{dt} \quad (1)$$

$$-UA(T_r - T_h) - \Delta H_{20\text{-}60C}\, 2kC_{A0}e^{(-kt)}\, V = \rho V C_p \frac{dT_r}{dt} \quad (2)$$

in which:

				Remarks:
U	Heat transfer coefficient	0.25	[kW/m^2/^{0}C]	(approximate value based on the value given in PSD ST4511)
A	Heat exchange area	2.6675	[m^2]	refer to appendix A5.3 of reactor design
T_r	Temperature in the reactor	20-60	[^{0}C]	The raw materials at 20^{o}C when added into the reactor and then the reaction mixture is heated to 60^{o}C
T_h	Temperature of hot steam	110	[^{0}C]	Refer to part 5.5, chapter 5
$\Delta H_{20\text{-}60C}$	Average reaction enthalpy from 20-60^{o}C	-62,755	[kJ/kmol]	Calculated from enthalpy data in A4.1 (batch remarks and calculations) and stoichiometry

k	Reaction constant	1.5351	[h^{-1}]	Calculated previously in this appendix
C_{Ao}	Initial reactant concentration (R-enantiomer)	0.1801	[$kmol/m^3$]	(calculated from mass balance)
ρ	Mol density of reaction mixture	9.39	[$kmol/m^3$]	(calculated from mass balance based on the volume of reaction mixture)
V	Volume of reaction mixture	0.667	[m^3]	Refer to appendix A5.3
C_p	Heat capacity of reaction mixture	155.13	[$kJ/kmol/^0C$]	(calculated from data in table 4.2 of chapter 4 and stoichiomety in appendix A4.1 of batch remarks and calculation)
t	Heating time	-	[h]	

Solving equation (2) by using RRSTIFF software gives:
$T_r = 60^0C$, t = 0.212 hours = 12.72 min.

Total amount of heat needed for reaction mixture is:
$H = \rho V C_p(T_r - T_{r0}) + \Delta H_{20\text{-}60C} 2V(C_{A0} - C_A)$ = 38869.7- 4184.94 = 34684.8kJ.

Using the heat of condense of steam = 2200kJ/kg
→ *The total amount of steam needed is H/2200 = 15.77kg*

c) *<u>Heat balance during the reaction (the temperature is maintained at 60°C)</u>*

After the temperature in the batch reactor reaches 60 ^{0}C, steam of hot steam is switched off.
Because the reaction is exothermal reaction (refer to chapter 4 of thermodynamic properties), cooling water is needed to maintain the temperature in the reactor at 60°C.

Heat balance for reaction mixture and cooling water:

$$0 = F_c C_{p,c}\left(T_{c_0} - T_c\right) + UA\left(T_r - T_c\right) \quad (3)$$

$$0 = V(\Delta H_{r60C}) 2k_0 C_{A0} e^{(-k_0 t)} - UA\left(T_r - T_c\right) \quad (4)$$

From equation (4):

$$\rightarrow T_C = \frac{-1}{UA}\left[V\Delta H_{r60C}\, 2k_0 C_{A0} e^{(-k_0 t)}\right] + T_r \quad (5)$$

From equation (3)

$$\rightarrow F_C = \frac{-UA\left(T_r - T_C\right)}{C_{P,c}\left(T_{C0} - T_C\right)} \quad (6)$$

Put T_c in equation (5) into equation (6):

$$\rightarrow F_C = \frac{-\left[V\Delta H_{r60C}\, 2k_0 C_{A0}{}' e^{(-k_0 t)}\right]}{C_{P,c}\left(T_{C0} + \frac{1}{UA}\left[V\Delta H_{r60C}\, 2k_0 C_{A0}{}' e^{(-k_0 t)}\right] - T_r\right)} \quad (7)$$

in which:

				Remarks:
U	Heat transfer coefficient	0.25 ×3600	[$kW/h/m^2/^0C$]	(approximate value based on the value given in PSD ST4511)
A	Heat exchange area	2.6675	[m^2]	refer to appendix A5.3 of reactor design
T_r	Temperature in the reactor	60	[^0C]	The reaction mixture is maintained at 60^oC during reaction
T_{co}	Initial temperature of cold water	20	[^0C]	Refer to part 5.5
T_c	Temperature of cold water		[^0C]	
ΔH_{20-60C}	Average reaction enthalpy at 60^oC	62,480	[kJ/kmol]	Calculated from enthalpy data in A4.1 (batch remarks and calculations) and stoichiometry
k	Reaction constant	1.5351	[h^{-1}]	Calculated previously in this appendix
C_{Ao}	Reactant concentration (R-enantiomer) when cooling starts	0.1301	[$kmol/m^3$]	(calculated from mass balance, reaction time and formula: $C_{A0}' = C_{A0} exp(-k_0 t)$. t = 0.212h, which is the heating time needed)
V	Volume of reaction mixture	0.667	[m^3]	Refer to appendix A5.3
C_p	Heat capacity of cooling water	4.18	[$kJ/kg/^0C$]	Data from instruction manual of the course CPD (ST4931)
F_c	Flow rate of cooling water		[kg/h]	
t	Cooling time		[h]	

The time t changes from 0 - 4.238h = total reaction time (4.5h) - heating time (0.212h)

The flow rate of cooling water is calculated using equation 7:
$\rightarrow F_c$ changes from 120.43kg/h to 0 kg/h.

Total amount of heat needed to transfer is $H = V \times 2 \times C_{A0} \times \Delta H_{60C} = 10843.6kJ$. Integrate equation (7) from 0 to 4.238 h, it is found that *71.48kg of total cooling water are needed.*

d) *<u>Heat balance when cooling down the reaction mixture</u>*

After 4.5 h of reaction time (including heating time), the conversion degree is 99.9%. Cooling water is used to cool down the reaction mixture from 60^0C to 30^0C. The cooling water temperature ranges from 20^0C to 25^0C.

It is also possible to cool the mixture to 25^0C or even lower but it will take longer time and more cooling water needed (see table A4.3 below). 30^0C is acceptable for the temperature of the liquid running through pipe, so 30^0C is chosen as temperature for the reaction mixture at reactor exit (option 2 in table A4.3)

Table A4.3: The options for the temperature at reactor exit and amount of cooling water needed

Option	*Time needed (h)*	*Amount of cooling water (kg)*	*Remarks*
1	0.723	581.15	Cool the liquid to 35C^o and outlet temperature of cooling water is 30C^0
2	0.787	1394.77	Cool the liquid to 30C^0 and outlet temperature of cooling water is 35C^0
3	1.03	4068.07	Cool the liquid to 25C^0 and outlet temperature of cooling water is 22C^0
4	1.48	8833.51	Cool the liquid to 22C^0 and outlet temperature of cooling water is 21C^0

Assume reaction does not occur during cooling down period.

Heat balance:

Heat transfer = Temperature hold up

$$UA(T_r - T_c) = \rho V C_p \frac{dT_r}{dt} \tag{8}$$

				Remarks:
U	Heat transfer coefficient	0.25	[kW//m^2/^{0}C]	(approximate value based on the value given in PSD ST4511)
A	Heat exchange area	2.6675	[m^2]	refer to appendix A5.3 of reactor design
T_r	Temperature in the reactor	60-30	[^{0}C]	The reaction mixture is cooled down from 60^{o}C to 30^{o}C
T_c	Temperature of cold water	25	[^{0}C]	(high temperature of cold water is chosen for worst case in a hot summer day)
ρ	Mol density of reaction mixture	9.39	[kmol/m^3]	(calculated from mass balance based on the volume of reaction mixture)
V	Volume of reaction mixture	0.667	[m^3]	Refer to appendix A5.3
C_p	Heat capacity of reaction mixture	155.13	[kJ/kmol/^{0}C]	(calculated from data in table 4.2 of chapter 4 and stoichiometry in appendix A4.1 of batch remarks and calculation)
t	Cooling time		[h]	

Equation (8) is solved using RRSTIFF program
$\rightarrow T_r = 30^0$C, t = 0.7875 h = 48min.

Total amount of heat need to removed from reaction mixture is
$H = \rho V C_p(T_{r0}-T_r) = 29146.1$ kJ

The temperature difference of cooling water is 10 ^{0}C (=35-25), and C_p = 4.18kJ/kg ^{0}C.
$\rightarrow$ *The total amount of cooling water needed is H/10/4.18 = 697.3kg*

A4.3.2 Distillation column C101

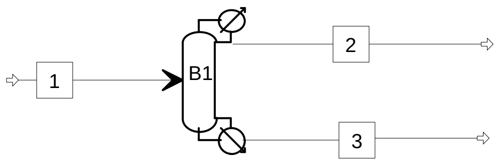
a) *<u>Heat and material balance of distillation column C101</u>*
(calculated using ASPEN PLUS simulation engine)

The calculation in distillation column is done in ASPEN PLUS simulation engine.

The procedure is explained as the following:

- One of the column models in ASPEN is DSTWU. DSTWU is primarily used to predict parameters, which are going to be used in more rigorous model (RADFRAC model in ASPEN).
- The feed stream is then inputted in DSTWU. Number of stages is guessed first. Light key, heavy key, and each desired recovery rate are inputted as well. Condenser and reboiler pressure are also needed to run the simulation in DSTWU.
- After all required inputs are completed, the simulation can be run.
- Once the simulation is done, the results, i.e.: minimum and actual reflux ratio, minimum and actual number of stages, distillate to feed ratio, can be obtained.
- If the requirement is met (in term of purity of product), then the simulation in RADFRAC column can be started.
- In RADFRAC, the results from DSTWU are used.
- In RADFRAC, more rigorous calculation is done. If the requirement is met, then the results can be used.

Herewith, the result of simulation is presented:



Number of stages: 22
Feed stage: 10
Reflux ratio: 0.45

<u>Table A4.4</u>: Operating conditions of distillation column

Pressure	top	0.15 atm
	bottom	0.15 atm
Temperature	top	307.1 K
	bottom	373.2 K
Heat duty	top	-121.022 kW
	bottom	102.202kW

The heat and mass balance can be seen in the following table:

Table A4.5: Heat and material balance of distillation column

Heat and Material Balance Table				
Stream ID		1	2	3
From			B1	B1
To		B1		
Phase		LIQUID	LIQUID	LIQUID
Substream: MIXED				
Mole Flow	kmol/sec			
PROPENEA		4.17926E-5	4.17926E-5	1.4950E-12
PERCURSO		8.32645E-5	2.59115E-7	8.30054E-5
REACTANT		1.04794E-7	4.9870E-32	1.04794E-7
ACETO-01		8.33333E-5	8.33333E-5	1.5889E-19
TOLUE-01		1.96001E-3	1.95964E-3	3.63124E-7
WATER		9.39018E-6	9.39018E-6	2.8428E-35
ISOPR-01		1.87755E-5	1.87755E-5	3.9970E-23
Total Flow	kmol/sec	2.19667E-3	2.11319E-3	8.34733E-5
Total Flow	kg/sec	.2086400	.1909392	.0177008
Total Flow	cum/sec	2.54095E-4	2.23392E-4	1.47166E-5
Temperature	K	361.2611	307.1058	373.1691
Pressure	N/sqm	1.01325E+5	15198.75	15198.75
Vapor Frac		0.0	0.0	0.0
Liquid Frac		1.000000	1.000000	1.000000
Solid Frac		0.0	0.0	0.0
Enthalpy	J/kmol	-1.5714E+7	-8.8267E+6	-4.1553E+8
Enthalpy	J/kg	-1.6544E+5	-97688.11	-1.9596E+6
Enthalpy	Watt	-34518.34	-18652.48	-34686.05
Entropy	J/kmol-K	-3.2599E+5	-3.3631E+5	-7.7383E+5
Entropy	J/kg-K	-3432.229	-3722.018	-3649.232
Density	kmol/cum	8.645060	9.459582	5.672034
Density	kg/cum	821.1107	854.7280	1202.778
Average MW		94.98033	90.35579	212.0541
Liq Vol 60F	cum/sec	2.33711E-4	2.19938E-4	1.37735E-5

b) *Heat needed (released) and utilities needed for different heat exchangers*

There are three heat exchanges in distillation process, which are feed heater, reboiler, and condenser (please refer to Process Flow Scheme, figure 5.1, chapter 5)

b1) *Reboiler*

Table A4.6: Amount of steam needed for reboiler

Heat needed for reboiler 102.2 kW 367,927.2 kJ/h	*Flow temperature* (^oC) Inlet 98.2 Outlet 100.01 (temp. at 22nd stage of distillation column)
Mass of steam (if using HP steam 225^o C 25bar) 167.24 kg/h	
Mass of steam (if using LP steam 110^o C 1.5bar) 167.24 kg/h	
Remarks: Heat of condense of all steams are 2200 kJ/kg HPS is more expensive than LPS so LP steam is chosen (refer to part 5.5 for utilities chosen) Heat needed for reboiler get from ASPEN simulation (refer to table A4.4) Inlet flow temperature from ASPEN simulation (temp. at 21st stage of distillation column) Outlet flow temperature from ASPEN simulation (refer to table A4.4)	

Note that mass of steam is calculated as:

$$\text{Mass of steam} = \frac{Heat\ needed}{Heat\ of\ condense} = \frac{367,927.2\frac{kJ}{h}}{2200\frac{kJ}{kg}} = 167.24\frac{kg}{h}$$

b2) *Condenser*

Table A4.7: Amount of cooling water needed for condenser

Heat released to condenser 121.022 kW (-) 435,679.2 kJ/h	*Flow temperature* (^oC) Inlet 53.7 Outlet 34
Mass of cooling water (temperature range: 20-30^{0}C) 10422.95 kg/h 2.90 kg/s	
Remarks: Heat released for condenser get from ASPEN simulation (refer to table A4.4) Inlet flow temperature from ASPEN simulation (at the 2nd stage of distillation column) Outlet flow temperature from ASPEN simulation (refer to table A4.5) Heat capacity of water is 4.18 kJ/kg-C (Data from instruction manual of the course ST4931) Assuming cooling water temperature difference is 10^{0}C	

Note that mass of cooling water is calculated as:

$$\text{Mass of cooling water} = \frac{Heat\ released}{Heat\ Capacity \times Temperature\ difference}$$

$$= \frac{435,679.2\frac{kJ}{h}}{4.18\frac{kJ}{kg\,^oC}\left(30-20\right)\,^oC} = 10422.95 kg/h = 2.90 \text{ kg/s}$$

b3) Heater for feed flow

Table A4.8: Heat capacity of the components of the feed to the distillation column

Components	*Heat capacity (kJ/kmolK)*	*Feed flow (kmol/h)*	*Fractional heat capacity (kJ/kmolK)*
Propenyl acetate	181.1178	0.1505	3.446875
Precusor	224.987	0.2998	8.529369
Racemic mixture	156.4094	0.0004	0.007911
Acetone	122.4175	0.3000	4.644004
Toluene	152.9257	7.0560	136.4479
Water	69.32727	0.0338	0.296312
Isopropanol	172.2369	0.0676	1.472315
Total		7.9081	154.8447

Remarks:
- Heat capacity of the components are obtained from ASPEN simulation engine (refer also to chapter 4 of thermodynamic properties)
- Feed flow is from mass balance (calculated from results in table A4.5)

$$Fractional\ heat\ capacity = \frac{Heat\ capacity \times Feed\ flow(of\ component)}{Total\ feed\ flow}$$

Heat needed to heat the feed is calculated as: $\Delta H = Cp\ m\Delta T$
where:

ΔH	heat needed for feed flow		[kW]
Cp	fractional heat capacity	154.8447	[kJ/kmolK]
m	total number of mol of feed per hour	7.9081	[kmol/h]
ΔT	Temperature difference	60	[^{0}C or K]

→ $\Delta H = 154.8447 \times 7.9081 \times 60 = 83267.86$kJ/h = 23.13 kW.

→ $\Delta H_{\text{from ASPEN}} = 25.201$ kW

Comment: in this calculation, the average heat capacity is used to compute the heat needed for feed flow. The average heat capacity is calculated by merely averaging the heat capacity at initial temperature and that at final temperature. The calculation is also done in ASPEN. However the results are a bit different, because in ASPEN, the heat capacity is a function of temperature. In the next calculation, the result from ASPEN is used.

The amount of steam needed to heat the feed is presented in table A4.9 below.
- If the condensate of HP steam from the reboiler is used, the outlet temperature of the condensate is calculated as:

$$Outlet\ temperature = Inlet\ temperature - \frac{Heat\ needed\ to\ heat\ the\ feed}{Heat\ Capacity \times Amount\ of\ condensate}$$

$$Outlet\ temperature = 225 - \frac{90,273.6}{4.18 \times 167.24} = 95.86\ ^0C$$

- If LP steam is used as heating medium, the mass of LP steam needed is calculated as:

$$Mass\,of\;LP\,steam\,needed = \frac{Heat\;needed\,to\,heat\,the\;feed}{Heat\;of\;condense} = \frac{90,273.6}{2200} = 41.03\frac{kg}{h}$$

Table A4.9: Amount of steam needed to heat the feed fed to distillation column

Heat needed for feed 25.201 kW 90,273.6 kJ/h	*Flow temperature* Inlet 20 ^{0}C Outlet 88 ^{0}C
Heating medium: condensate of HP steam from the reboiler Outlet temperature of Condensate 95.86 ^{0}C	 Mass of condensate of HP steam from the reboiler 167.24 kg/h
Heating medium: low pressure steam 41.03 kg/h	
Remarks: - Heat needed to heat the feed is calculated above - Inlet flow temperature of the feed to the distillation column is the same as the temp. of the liquid in intermediate storage tank (refer to part 3.2.2, chapter 3) - Outlet flow temperature is obtained from table A4.5 - Mass of condensate of HP steam from the reboiler is from table A4.6 - Heat of condense of all steams are 2200 kJ/kg	

b4) Product cooler

Heat released to the cooler is calculated as: ΔH = Cp mΔT
where:

Cp	heat capacity of product	224.987	[kJ/kmolK]
m	number of mol of product	0.2998	[kmol/h]
ΔT	Temperature difference	73.2 (=98.2 –25)	[^{0}C or K]

→ ΔH = 224.987 × 0.2998 × 73.2 = 4937.42 kJ/h = 1.37 kW.

→ $\Delta H_{\text{from ASPEN}}$ = 1.55 kW

Table A4.10: Amount of cooling water needed for product cooler

Heat released to the cooler 5583.6 kJ/h 1.55 kW	Flow Temperature 98.2 ^{0}C 25 ^{0}C
Mass of cooling water (temperature ranges from 20-30^{o}C) 133.58 kg/h	 0.0371 kg/s
Remarks: - Outlet temperature is 25^{0}C (designed assumption) - Inlet temperature gets from ASPEN simulation (temp. at 21st stage of distillation column) - Heat released to the cooler is obtained from calculation above - Heat capacity of water is 4.18 kJ/kg-C (Data from instruction manual of the course ST4931)	

Using the same formula as in *b2* (formula to calculate the amount of cooling water needed for the condenser), mass of cooling water needed for product cooler is determined to be 133.58 kg/h

A4.3.3 The possibilities of pinch technology

1. *Pinch reaction part and separation part*

It is impossible because the reactor part is batch process and the distillation column operates continuously and the working schedules are different. Therefore it is not possible to do pinch between these two parts. Therefore, only in separation part, pinch technology is considered since it operates continuously.

2. *Possibilities of pinch technology in separation part*

<u>Using feed flow as cold utility for condenser</u>

Because the heat needed to heat the feed fed to distillation column is 25.2 kW and the heat released to condenser is 121.022 kW. If feed fed to distillation column is used as cold utility for condenser, it means that extra cold utility will be needed to cool the condenser therefore extra heat exchanger is required.

In addition, the maximum temperature in condenser is only 53.7^{o}C, but the temperature of feed fed to distillation column should reach 88^{0}C. It means extra hot utility should be used to heat feed flow from 45^{0}C (this number is just appraised) to 88^{0}C. As a result, one more heat exchanger is needed.

Although using pinch technology here can save a little amount of steam and cooling water, but it will require two more heat exchangers. Since the heat exchangers cost much more than the saving on utilities (steam and cooling water) so it is not worth to use feed flow fed to distillation column as cold utility for condenser.

<u>Using HP steam to heat reboiler and then using the condensate of HP steam from reboiler to heat feed fed to distillation column</u>

This combination is a possibility, however, it is not chosen because using 2 streams of LP steam to heat reboiler and feed flow separately is more economical. The comparison of these 2 different combinations is shown below.

- If high-pressure steam is chosen:

<u>Table A4.11</u>: Comparison of outlet temperature of condensate using different kinds of HP steam

Types of steam	*Pressure (bar)*	*Temperature (^{0}C)*	*Outlet temperature of condensate (^{0}C)*	*Possibility*
1	25	225	95.86	Yes
2	18	205	86	No
3	4	140	21	No
Remarks: - The outlet temperature of the condensate is calculated using the formula in b3				

It is shown from table A4.11 that 25 bar 225 ^{0}C steam is the only HPS can be used for reboiler and heater because the outlet temperature is high enough to fit the required temperature of the feed of the distillation column (need to be heated to 88^{0}C).

The amount of LP steam required for reboiler and for heating feed to distillation column is 208.27 kg/h (= 167.24 + 41.03) (refer to tables A4.6 and A4.9)

If HP steam is used for reboiler and then the condensate is used to heat the feed to distillation column 167.24 kg/h HP steam is needed. Since the difference of the amount is only 41.03 kg, and also the price of HP steam is much higher than LP steam, therefore 2 streams of LP steam to heat reboiler and feed flow separately are used

The types and the amount of utilities used for the heating and cooling systems in distillation column is summarized in the table below

Table A4.12: The types and the amount of utilities used for the heating and cooling systems in distillation column

	Heat transferred (kW)	*Inlet temperature (^0C)*	*Outlet temperature (^0C)*	*Utility type*
Reboiler	102.20	98.0	100.02	LP steam
Condenser	121.02	54.0	34.0	Cooling water
Feed heater	25.20	20.0	88.0	LP steam
Product cool	1.55	98.2	25.0	Cooling water

APPENDIX A5 PROCESS AND EQUIPMENT DESIGN

A5.1 Design of storage tanks T101, T104 and T105

A5.1.1 Toluene storage tank T101

Assumption: - toluene storage tank can stores the amount of toluene required for 20 batches

The amount of toluene required for each batch is 520.1kg (part 5.4 chapter 5)
The density of toluene is 0.866 g/cm^3 or 0.866 × 10^3 kg/m^3 (part 3.2.4, chapter 3)
→ The volume of toluene is 520/0.866 × 10^3= 0.602m^3/batch
The total volume required for 20 batches is 0. 602m^3/batch × 20 batches = 12m^3
It is designed that the liquid only occupies 80% of the volume of the tank (for safety reason), so the total design volume is 15.1m^3.

The diameter of the tank is chosen to be 2m and by using the following equation $V = \frac{\pi}{4} D^2 H$, the height of tank is calculated to be 4.8m.

A5.1.2 Technical grade toluene's storage tank T104

This tank is used to store the by-product technical grade toluene of 1 production year, which is 55 tons (table 3.7, chapter 3)
Assume that the density of technical grade toluene is also 0.866 g/cm^3 or 0.866 × 10^3 kg/m^3
→ The volume of technical grade toluene is 55,000/0.866 × 10^3 = 63.5m^3
It is designed that the liquid only occupies 80% of the volume of the tank (for safety reason), so the total design volume is 79.4m^3.

The diameter of the tank is chosen to be 3m and by using the following equation $V = \frac{\pi}{4} D^2 H$, the height of tank is calculated to be 11.2m.

A5.1.3 Product storage tank T105

This tank is designed for enough storage of product produced in 1 production year, which is 5095kg (table 3.6, chapter 3)

The density of the product is 1.5121 g/cm^3 or 1512kg/m^3 (part 3.2.4, chapter 3)
→ The volume of product is 5095/1512 × 10^3 = 3.4m^3

It is designed that the liquid only occupies 80% of the volume of the tank (for safety reason), so the total design volume is 4.2m^3.

The diameter of the tank is chosen to be 1.5m and by using the following equation $V = \frac{\pi}{4} D^2 H$, the height of tank is calculated to be 2.4m.

A5.10 The simulation (ASPEN PLUS model) in the process of producing the precursor of Prozac, 3-chloro-1-phenylpropyl acetate

In the process of producing precursor, Aspen plus is used to simulate the operation of distillation column.

In the feed stream, it is a mixture of the following chemical substances:

Precursor of Prozac:	3-chloro 1-phenylpropyl acetate.
Reactant 1:	3-chloro-1-phenyl –1- propanol
Reactant 2:	Propenyl acetate
By-product of reaction:	Acetone
Solvent:	Toluene
By-product of precipitation:	Isopropyl alcohol (isopropanol)

But in the data bank of Aspen plus, there is no chemical substance of *reactant 1* and *precursor*, and physical properties as well. So, first the substance has be defined and the method has to be chosen to estimate the physical properties.

- For the *reactant 1*, the name is defined as “reactant” and the formula is $C_9H_{11}OCl$. “Unifac group contribution method” and “Joback group contribution method” were chosen to estimate the physical properties, because “Joback group contribution method” can be used to estimate the properties as boiling point, enthalpy of formation, entropy of formation, heat capacity etc. of pure substance, and “Unifac group contribution method” can be used to estimate activity coefficient and all thermodynamics properties of mixture. These two methods are mostly used to estimate physical properties in the Aspen plus.

Table A5.10.1: Unifac group contribution method for reactant

Unifac group contribution method	
Group number	Number of occurrences
2010	1
1200	1
1010	1
1150	1
1105	5

Table 5.10.2: Joback group contribution method for reactant

Joback group contribution method	
Group number	Number of occurrences
113	5
114	1
102	1
119	1
116	1
101	2

- For the *precursor of Prozac*, the name is defined as “precursor” and the formula is $C_{11}H_{13}O_2Cl$. “Unifac group contribution method” and “Joback group contribution method” is chosen to estimate the physical properties of substances. The reason is same as the explained above.

Table A5.10.3: Unifac group contribution method for the precursor

Unifac group contribution method	
Group number	Number of occurrences
1010	1
1150	1
1105	5
1505	1
2010	1

Table 5.10.4: Joback group contribution method for precursor

Joback group contribution method	
Group number	Number of occurrences
100	1
101	2
102	1
113	5
116	1
127	1
114	1

Then all the chemical substances are defined or found in the data form of components specification as followed (See aspen file):

PROPENEA	CONV	ETHYL-ACRYLATE	C5H8O2
PERCURSO	CONV		C11H13O2CL
REACTANT	CONV		C9H11OCL
ACETO-01	CONV	ACETONE	C3H6O-1
TOLUE-01	CONV	TOLUENE	C7H8
WATER	CONV	WATER	H2O
ISOPR-01	CONV	ISOPROPYL-ALCOHOL	C3H8O-2

Normally, RADFRAC model is chosen to simulate the distillation column operation. Because the RADFRAC model is for rigorously simulating distillation (also including absorption, stripping, extractive and azeotropic distillation), a lot of data such as reflux ratio, number of stages, etc is needed to start the simulation. In the starting period, such data is still missing. Aspen provide another simulation model DSTWU, to estimate the necessary data for rigorous calculation.

Hence, first DSTWU model is used to predict some basic parameter roughly:

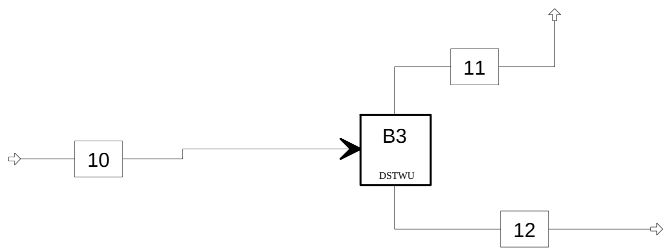


Figure 5.10.1: DSTWU simulation model in ASPEN PLUS

- In the stream 10, the following data is filled:

Component	Mass-flow(kg/hr)
PROPENEA	15.063
PERCURSO	63.75
REACTANT	0.051

ACETO-01	17.424
TOLUE-01	650.145
WATER	0.609
ISOPR-01	4.062

Pressure = 1 atm; Vapor fraction = 0

- In the block B3, the key component recoveries are filled:
  Toluene: 0.9999
  Precursor: 0.001
  Number of stages: 2
  Pressure of condenser:0.15 bar
  Pressure of reboiler:0.2 bar

(The above data is assumed as the calculation starting point; DSTWU model will give the calculation result)

- Then the DSTWU can start to simulate.

From the simulation result of DSTWU, the reflux ratio of 0.45 is obtained; the amount of stages is 22 (including condenser and reboiler); distillate to feed ratio is 0.962.

The detail data is as the following (See Aspen file):

Data Blocks B3 Output MIN_REFLUX	0.27526901	
Data Blocks B3 Output **ACT_REFLUX**	**0.4464013**	
Data Blocks B3 Output MIN_STAGES	10.5846429	
Data Blocks B3 Output **ACT_STAGES**	**21.1692859**	
Data Blocks B3 Output FEED_LOCATN	10.2627014	
Data Blocks B3 Output RECT_STAGES	9.26270136	
Data Blocks B3 Output REB_DUTY	96759.6608	Watt
Data Blocks B3 Output COND_DUTY	115297.534	Watt
Data Blocks B3 Output DISTIL_TEMP	307.097452	K
Data Blocks B3 Output BOTTOM_TEMP	384.983597	K
Data Blocks B3 Output **DIST_VS_FEED**	**0.96199602**	

With these data, use the model RADFRAC for rigorous calculation:

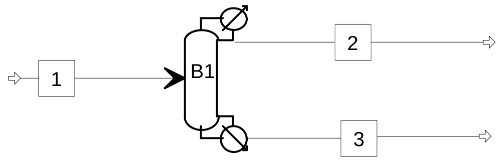


Figure A5.10.2: RADFRAC simulation model in ASPEN PLUS

- The input in the stream 1 is the same as in stream 10 above. In the block B1, the following data is input:
  Number of stages: 22
  Reflux ratio: 0.45
  Distillate to feed ratio: 0.962
  Feed stage:10
  Pressure 0.15bar
  Condenser: total

- Then the model RADFRAC starts to simulate.

Table A5.10.5: The simulation result of RADFRAC

Substream: MIXED	1	2	3
Mole Flow kmol/sec			
PROPENEA	4.18E-05 kmol/sec	4.18E-05 kmol/sec	1.50E-12 kmol/sec
PERCURSO	8.33E-05 kmol/sec	2.59E-07 kmol/sec	8.30E-05 kmol/sec
REACTANT	1.05E-07 kmol/sec	4.99E-32 kmol/sec	1.05E-07 kmol/sec
ACETO-01	8.33E-05 kmol/sec	8.33E-05 kmol/sec	1.59E-19 kmol/sec
TOLUE-01	0.00196 kmol/sec	0.00196 kmol/sec	3.63E-07 kmol/sec
WATER	9.39E-06 kmol/sec	9.39E-06 kmol/sec	2.84E-35 kmol/sec
ISOPR-01	1.88E-05 kmol/sec	1.88E-05 kmol/sec	4.00E-23 kmol/sec
Total Flow kmol/sec	0.00219666 kmol/sec	0.002113 kmol/sec	8.35E-05 kmol/sec
Total Flow kg/sec	0.20864 kg/sec	0.190939 kg/sec	0.017701 kg/sec
Total Flow cum/sec	0.00025409 cum/sec	0.000223 cum/sec	1.47E-05 cum/sec
Temperature K	361.261064 K	307.1058 K	373.1691 K
Pressure N/sqm	101325 N/sqm	15198.75 N/sqm	15198.75 N/sqm
Density kmol/cum	8.64506041 kmol/cum	9.459582 kmol/cum	5.672034 kmol/cum
Density kg/cum	821.110659 kg/cum	854.728 kg/cum	1202.778 kg/cum
Average MW	94.980328	90.35579	212.0541
Liq Vol 60F cum/sec	0.00023371 cum/sec	0.00022 cum/sec	1.38E-05 cum/sec

From the above table, the product purity can be calculated: 99.4%(mol), which satisfies the requirement. So, the above result can be used as the base of the column design. The detail of designing column is in appendix A5.7.

A5.11 Equipment data sheets

A5.11.1 Equipment data summary sheets

Table A5.11.1: Data summary sheet of storage tanks and vessels T101-T103 & V101

STORAGE TANKS AND VESSELS – DATA SUMMARY SHEET				
EQUIPMENT NUMBER: **NAME:**	**T101** *Toluene storage tank*	**T102** *Dissolving tank*	**V101** *Buffer tank*	**T103** *Precipitation tank*
	Vessel	Vessel	Vessel	Vessel
Pressure [bar]	1	1	1	1
Temperature [°C]	20.0	20.0	20.0	30.0
Volume [m^3] (1)	15.1	0.75	0.4	0.84
Diameter [m]	2	1	0.65	1
L or H [m]	4.8	0.96	1.45	1.07
Internals				
-Stirrer type	n.a	Impeller	n.a	Impeller
-Stirrer diameter [m]	n.a	0.33	n.a	0.33
-Stirrer height [m]	n.a.	0.042	n.a.	0.042
-Power needed [kW]	n.a	0.15	n.a	0.17
-Well-mixing time [s]	n.a	106.3	n.a	115
Number **-Series:**	1	1	1	1
- Parallel:	-	-	-	-
Materials of construction (2)	CS	CS	CS	CS
Other:				

Remarks:
(1) The effect volume of vessel is 20% of total volume.
(2) SS = Stainless Steel; CS = Carbon Steel

Table A5.11.2: Data summary sheet of storage tanks and vessels V102-V103 & T104-T105

STORAGE TANKS AND VESSELS - DATA SUMMARY SHEET				
EQUIPMENT NUMBER: **NAME:**	**V102** *Intermediate storage tank*	**V103** *Buffer tank*	**T104** *Technical grade toluene storage tank*	**T105** *Product storage tank*
	Vessel	Vessel	Vessel	Vessel
Pressure [bar]	1	0.15/0.15	1	1
Temperature [°C]	30.0/20.0	34.0	34.0/20.0	25.0
Volume [m^3] (1)	16.75	1.44	79.4	4.2
Diameter [m]	2.5	1	3	1.5
L or H [m]	3.5	1.84	11.2	2.4
Internals				
-Stirrer type	n.a	n.a	n.a	n.a
-Stirrer diameter [m]	n.a	n.a	n.a	n.a
-Stirrer height [m]	n.a.	n.a.	n.a.	n.a.
-Power needed [kW]	n.a	n.a	n.a	n.a
-Well-mixing time [s]	n.a	n.a	n.a	n.a
Number				
-Series	1	1	1	1
- Parallel	-	-	-	-
Materials of construction (2)	CS	CS	CS	CS
Other				

Remarks:
(1) The effect volume of vessel is 20% of total volume.
(2) SS = Stainless Steel; CS = Carbon Steel

Table A5.11.3: Data summary sheet of reactor R101

REACTOR R101 - DATA SUMMARY SHEET			
EQUIPMENT NUMBER: **NAME:**	**R101** *Batch Jacketed Reactor*		
	Vessel	Jacket (1)	
Pressure [bar]	1	1	1.5
Temperature [°C]	30.0	20/25	100 /110
Volume [m^3] (2)	0.84		
Heat transfer area [m^2]		3.334	
Diameter [m]	1		
L or H [m]	1.07		
Internals			
-Stirrer type:	Impeller		
-Stirrer diameter [m]	0.33		
-Stirrer height [m]	0.042		
-Power needed [kW]	0.17		
-Well-mixing time [s]	115		
Number			
-Series	1	1	
- Parallel	-	-	
Materials of construction (3)	CS	Al-Br	
Other			

Remarks:
(1) In jacket the first column is for cooling water, second column is for L.P steam.
(2) The effect volume of vessel is 20% of total volume.
(3) SS = Stainless Steel; CS = Carbon Steel, Al-Br = Aluminum Bronze

Table A5.11.4: Data summary sheet of distillation column C101

DISTILLATION COLUMN C101 - DATA SUMMARY SHEET	
EQUIPMENT NUMBER: **NAME:**	**C101** *T/P Splitter*
	Tray Column
Pressure [bar]	0.15/0.15
Temperature [°C]	34.0/100.0
Volume [m^3]	2.86
Diameter [m]	0.5
L or H [m]	14.55
Internals **-Tray type** **-Tray number** **-Fixed packing** **Type :** **Shape :** **-Catalyst** **Type :** **Shape :**	 Sieve Trays 20 n.a. n.a n.a. n.a.
Number **-Series :** **- Parallel :**	 1 -
Materials of construction (1)	Trays: SS314 Column: CS
Other	
Remarks: (1) SS = Stainless Steel; CS = Carbon Steel	

Table A5.11.5: Data summary sheet of heat exchangers E101-E104

HEAT EXCHANGERS - DATA SUMMARY SHEET				
EQUIPMENT NUMBER **NAME**	**E101** *C101 feed heater*	**E102** *C101 Condenser*	**E103** *C101 Reboiler*	**E104** *Product cooler*
	Single tube Sheet	Single tubes Water cooled	Single tube Sheet	Single tubes Water cooled
Substance **-Tubes:** **-Shell:**	Toluene L.P. Steam	Toluene Cooling water	Precursor L.P. Steam	Precursor Cooling water
Duty [kW]	25.201	121.022	102.202	1.551
Heat exchange area [m^2]	2.1	26.27	37.63	0.26
Number **-Series** **- Parallel:**	1 -	1 -	1 -	1 -
Pressure [bar] **-Tubes** **-Shell**	1.0 1.5	0.15 1.0	0.15 1.5	1.0 1.0
Temperature In / Out [^oC] **- Tubes** **- Shell**	20.0 / 88.0 110.0 / 110.0	53.7 / 34.0 20.0 / 30.0	98.2/100.02 110.0 / 110.0	98.2/25 20.0/30.0
Special materials of construction (1)	Tubes : CS Shell : CS	Tubes : CS Shell : Al-Br	Tubes : CS Shell : CS	Tubes : CS Shell : Al-Br
Other				
Remarks: (1) CS = Carbon Steel; Al-Br = Aluminum Bronze				

Table A5.11.6: Data summary sheet of filters F101-F102

FILTERS - DATA SUMMARY SHEET				
EQUIPMENT NUMBER: **NAME:**	**F101** *Lipase B separation filter*	**F102** *La(OH)$_3$ separation filter*		
Type	Micro-Filter	Micro-Filter		
Pressure [bar]	1	1		
Temperature [°C]	30.0	30.0		
Average flux rate [l/m^{2}h]	20.0	20.0		
Power [kw/m^2]	0.2	0.2		
Maximum area [m^2]	80	80		
Internals **- Pump type:** **- Membrane replacement cost [operating hrs]** **-Unit membrane cost [$/m^2]**	 Centrifugal 2000 200	 Centrifugal 2000 200		
Number **- Series** **- Parallel**	 1 -	 1 -		
Materials of construction				
Other				

Remarks:

(1) The filters chosen from SUPERPRO design.
(2) Design the maximum membrane area as 80 m^2

Table A5.11.7: Data summary sheet of pumps P101-P104

PUMPS - DATA SUMMARY SHEET				
EQUIPMENT NUMBER: **NAME:**	**P101** *Toluene transport*	**P102** *Liquid transport*	**P103** *Liquid transport*	**P104** *C101 Feed transport*
Type **Number**	Centrifugal 2	Centrifugal 2	Centrifugal 2	Centrifugal 2
Medium transferred	Toluene	Toluene/ Catalyst	Toluene/ Product/ Catalyst…	Toluene/ Product/ water…
Capacity **[kg/s]** **[m^3/s]**	 0.866 0.001	 1.747 0.002	 0.500 5.5×10^{-4}	 0.212 2.4×10^{-4}
Density [kg/m^3]	866	873.6	904.5	897
Pressure [bar] **Suction / Discharge**	 0.94 /4.91	 0.94/3.59	 0.91 /3.71	 0.91 /3.71
Temperature In / Out [^{o}C]	20.0 / 20.0	20.0 / 20.0	30.0 / 30.0	20.0 / 20.0
Power [kW] **-Theoretical:** **-Actual:**	 0.4 1.5	 0.52 1.3	 0.15 0.7	 0.11 0.7
Number **-Theoretical:** **-Actual** (1)**:**	 2	 2	 2	 2
Special materials of construction:	MS casing	MS casing	MS casing	MS casing
Other	Double mechanical seals	Double mechanical seals	Double mechanical seals	Double mechanical seals
Remarks: (1) One installed spare included				

Table A5.11.8: Data summary sheet of pumps P105-P108

PUMPS - DATA SUMMARY SHEET				
EQUIPMENT NUMBER: **NAME:**	**P105** *C101 Vacuum*	**P106** *C101 Reflux*	**P107** *C101 Top*	**P108** *C101 Bottom*
Type **Number**	Rotary 2	Centrifugal 2	Centrifugal 2	Diaphram 2
Medium transferred	Air/Toluene	Toluene/Product	Toluene/Product	Product
Capacity **[kg/s]** **[m^3/s]**	 0.0096 0.008	 0.0855 1.0×10^{-4}	 0.188 2.2×10^{-4}	 0.018 1.5×10^{-5}
Density [kg/m^3]	1.2	854.7	854.7	1202.8
Pressure [bar] **Suction / Discharge**	0.14/ 3.27	0.297 / 2.359	0.201/ 3.99	0.6 / 4.8
Temperature In / Out **[^{o}C]**	34.0 / 34.0	34.0 / 34.0	34.0 / 34.0	25 .0/ 25.0
Power [kW] **-Theoretical:** **-Actual:**	 2.5 2.8	 0.021 0.11	 0.09 0.45	 0.0063 0.013
Number **-Theoretical:** **-Actual** (1)**:**	 2	 2	 2	 2
Special materials of construction:	MS casing	MS casing	MS casing	MS casing
Other	Double mechanical seals	Double mechanical seals	Double mechanical seals	Double mechanical seals

Remarks:
(1) One installed spare included

A5.11.2 Equipment data specification sheets

Table A5.11.9: Equipment data specification sheet of toluene/product splitter C101

DISTILLATION COLUMN C101 – DATA SPECIFICATION SHEET

EQUIPMENT NUMBER : C-101
NAME : Toluene/Product Splitter

General Data

Service : - distillation/ ~~extraction~~/ ~~absorption~~/ ——————
Column type : - ~~packed~~ / tray / ~~spray~~ / ——————
Tray type : - ~~cap~~—— / sieve / ~~valve~~ / ——————
Tray number (1)
- **Theoretical** : 22
- **Actual** : 20
- **Feed (actual)** : 9

Tray Distance (HETP) [m] : 0.45 **Tray Material: SS314** (2)
Column Diameter [m] : 0.5 **Column Material: CS** (2)
Column Height [m] : 14.55
Heating : - ~~none~~ /~~open steam~~ /reboiler/—————— (3)

Process Conditions

Stream Details	Feed		Top		**Bottom**		**Reflux / ~~Absorbent~~**		**~~Extractant~~ / ~~side stream~~**	
Temp. [^oC]	: 88		: 34		: 100		: 34			
Pressure [bara]	: 1.0		: 0.15		: 0.15		: 0.15			
Density [kg/m^3]	: 821.1		: 854.7		: 1202.8		: 854.7			
Mass Flow [kg/s]	: 0.209		: 0.191		:0.0177		: 0.086			
Composition	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**	**mol%**	**wt%**
Toluene	89.2	86.6	92.7	94.6	0.4	0.2	92.7	94.6		
Precursor	3.8	8.5	0.0	0.0	99.4	99.7	0.0	0.0		
Acetone	3.8	2.3	3.9	2.5	0.0	0.0	30.4	2.5		
Propenyl acetate	1.9	2.0	2.0	2.2	0.0	0.0	2.0	2.2		
Deionized water	0.4	0.1	0.4	0.1	0.0	0.0	0.4	0.1		
Isopropanol	0.9	0.5	0.9	0.6	0.0	0.0	0.9	0.6		

Column Internals (4)

Trays (5)
Number of ~~caps~~ / sieve holes / ——— : 693
Active Tray Area [m^2] : 0.136
Weir Length [mm] : 0.275
Diameter of chute pipe/hole/———————[mm] : 5

Packing *Not Applicable*
Type :
Material :
Volume [m^3] :
Length [m] :
Width [m] :
Height [m] :

Remarks:
(1) Tray numbering from top to bottom.
(2) SS = Stainless Steel; CS = Carbon Steel.
(3) Reboiler is E103; operates with LP steam.
(4) Sketch & measures of Column & Tray layout should have been provided.
(5) Tray layout valid for whole column.

Table A5.11.10: Equipment data specification sheet of batch jacketed reactor R101

BATCH JACKETED REACTOR R101– DATA SPECIFICATION SHEET				
EQUIPMENT NR. : **NAME:**	**R101** ***Batch Jacketed Reactor***		**Operating: 1** **Number: 1**	
Reactor		***Jacket*** (for different time scale)		
Pressure [bar]	1	**Pressure [bar]**	1 (cooling water)	1.5 (steam)
Temperature [°C]	20/60	**Temperature in/out [°C]**	20/25 (cooling water)	110/110 (steam)
Volume [m^3] (1)	0.84	**Heat exchange area [m^2]**	3.334	3.334
Diameter [m]	1	**Liquid height [m]**	0.849	0.849
L or H [m]	1.07	*Useful heat exchange are [m^2]*	2.668	2.668
Internals **-Stirrer type** **-Stirrer diameter [m]** **-Stirrer height [m]** **-Power needed [kW]** **-Well-mixing time [s]**	 Impeller 0.33 0.0416 0.168 115	**Heat transferred [kJ]** (2) **Time consuming [hrs]** (2)	10843.6(b) 29146.1(c) 4.238 (b) 0.788 (c)	34684.8(a) 0.212 (a)
Number **-Series** **- Parallel**	 1 -	***Number*** **-Series** **- Parallel**	 1 -	 1 -
Materials of construction (3)	CS	**Materials of construction** (4)	Al-Br	Al-Br
Other :				

Remarks:

(1) The effect volume of vessel is 20% of total volume.
(2) Duty (a) is for liquid heating, duty (b) is for temperature maintain, duty (c) is for liquid cooling.
(3) SS = Stainless Steel; CS = Carbon Steel
(4) Al-Br = Aluminum Bronze

Table A5.11.11: Equipment data specification sheet of distillation column's feed heater E101

DISTILLATION COLUMN'S FEED HEATER E101 – DATA SPECIFICATION SHEET					
QUIPMENT NUMBER	:	**E101**	**In Series**	:	1
NAME	:	***C101 Feed heater***	**In Parallel**	:	none
General Data					
Service	:	- **Heat Exchanger** - ~~**Cooler**~~ - ~~**Condenser**~~	- ~~**Vaporizer**~~ - ~~**Reboiler**~~		
Type	:	- ~~**Fixed Tube Sheets**~~ - ~~**Floating Head**~~ - ~~**Hair Pin**~~ - ~~**Double Tube**~~	- ~~**Plate Heat Exchanger**~~ - ~~**Finned Tubes**~~ - ~~**Thermosyphon**~~ - **Single Tube**		
Position	:	- ~~**Horizontal**~~ - **Vertical**			

Capacity	**[kW]**	:	25.02	*(1)*	**(Calc.)**
Heat Exchange Area	**[m^2]**	:	2.1	*(2)*	**(Calc.)**
Overall Heat Transfer Coefficient	**[$W/m^2\cdot{}^oC$]**	:	250		**(Approx.)**
Log. Mean Temperature Diff. (LMTD)	**[^oC]**	:	48.27	*(3)*	
Passes Tube Side		:	1		
Passes Shell Side		:	1		
Correction Factor LMTD (min. 0.75)		:	1.0		
Cor**rected LMTD**	**[^oC]**	:	48.27		

Process Conditions

			Shell Side	**Tube Side**
Medium		:	LP steam	Toluene/precursor
Mass Stream	**[kg/h]**	:	74.39	751.1040
Mass Stream to				
- Evaporize	**[kg/s]**	:	-	0
- Condense	**[kg/h]**	:	74.39	751.1040
Average Specific Heat	**[$kJ/kg\cdot{}^oC$]**	:	-	1.628
Heat of Evap. / Condensation	**[kJ/kg]**	:	2200	-
Temperature IN	**[^oC]**	:	110	20
Temperature OUT	**[^oC]**	:	110	88
Pressure	**[bar]**	:	1.5	1
Material *(4)*		:	CS	CS

Remarks:

(1) Capacity = Average Specific Heat × Total Amount of Feed

(2) Capacity = Area × Overall Heat Transfer Coefficient × LMTD

(3) $\Delta T_{lm} = \dfrac{(T_1 - t_2) - (T_2 - t_1)}{\ln \dfrac{(T_1 - t_2)}{(T_2 - t_1)}}$ **[15]** (p598 equation 12.4)

(4) CS = Carbon Steel

Table A5.11.12: Equipment data specification sheet of distillation column's reboiler E103

DISTILLATION COLUMN'S REBOILER E103 – DATA SPECIFICATION SHEET

EQUIPMENT NUMBER :	**E103**	**In Series :**	1
NAME :	***C101 Reboiler***	**In Parallel :**	none

General Data

Service	:	- ~~**Heat Exchanger**~~ - ~~**Cooler**~~ - ~~**Condenser**~~	- ~~**Vaporizer**~~ - **Reboiler**
Type	:	- ~~**Fixed Tube Sheets**~~ - ~~**Floating Head**~~ - ~~**Hair Pin**~~ - ~~**Double Tube**~~	- ~~**Plate Heat Exchanger**~~ - ~~**Finned Tubes**~~ - ~~**Thermosyphon**~~ - **Single Tube**
Position	:	- ~~**Horizontal**~~ - **Vertical**	

Capacity	**[kW]**	:	102.202	*(1)*	**(Calc.)**
Heat Exchange Area	**[m^2]**	:	37.63	*(2)*	**(Calc.)**
Overall Heat Transfer Coefficient	**[$W/m^2 \cdot {}^oC$]**	:	250		**(Approx.)**
Log. Mean Temperature Diff. (LMTD)	**[^oC]**	:	10.87	*(3)*	
Passes Tube Side		:	1		
Passes Shell Side		:	1		
Correction Factor LMTD (min. 0.75)		:	1.0		
Cor**rected LMTD**	**[^oC]**	:	10.87		

Process Conditions

			Shell Side	**Tube Side**
Medium		:	LP steam	Precursor
Mass Stream	**[kg/h]**	:	167.24	1205.93
Mass Stream to				
- Evaporize	**[kg/h]**	:	-	1205.93
- Condense	**[kg/h]**	:	167.24	-
Average Specific Heat	**[kJ/kg ^oC]**	:	1.88	
Heat of Evap. / Condensation	**[kJ/kg]**	:	2200	-
Temperature IN	**[^oC]**	:	110.0	98.2
Temperature OUT	**[^oC]**	:	110.0	100.02
Pressure	**[bar]**	:	1.5	0.15
Material *(3)*		:	CS	CS

Remarks:

(2) Heat capacity simulate from ASPEN

(3) Heat Capacity = Overall Heat Transfer Coefficient × Heat transfer Area × LMTD

(4) $\Delta T_{lm} = \dfrac{(T_1 - t_2) - (T_2 - t_1)}{\ln \dfrac{(T_1 - t_2)}{(T_2 - t_1)}}$ [15] (p598 equation 12.4)

(4)CS = Carbon Steel

Table A5.11.13: Equipment data specification sheet of distillation column's condenser E102

DISTILLATION COLUMN'S CONDENSER E102 – DATA SPECIFICATION SHEET

EQUIPMENT NUMBER :	**E102**	**In Series** :	1
NAME :	***C101 Overhead Condenser***	**In Parallel** :	none

General Data

Service	:	**- ~~Heat Exchanger~~ - ~~Vaporizer~~** **- ~~Cooler~~ - ~~Reboiler~~** **- Condenser (Water cooled)**
Type	:	**- ~~Fixed Tube Sheets~~ - ~~Plate Heat Exchanger~~** **- ~~Floating Head~~ - ~~Finned Tubes~~** **- ~~Hair Pin~~ - ~~Thermosyphon~~** **- ~~Double Tube~~ - Single Tube**
Position	:	**- Horizontal** **- ~~Vertical~~**

Capacity	**[kW]**	:	121.022	*(1)*	**(Calc.)**
Heat Exchange Area	**[m^2]**	:	26.27	*(2)*	**(Calc.)**
Overall Heat Transfer Coefficient	**[$W/m^2\ ^oC$]**	:	250		**(Approx.)**
Log. Mean Temperature Diff. (LMTD)	**[^oC]**	:	18.43	*(3)*	
Passes Tube Side		:	1		
Passes Shell Side		:	1		
Correction Factor LMTD (min. 0.75)		:	1.0	*(4)*	
Corrected LMTD	**[^oC]**	:	18.43		

Process Conditions

			Shell Side	**Tube Side**
Medium		:	Cooling water	Toluene / Precursor
Mass Stream	**[kg/s]**	:	2.90	0.2768
Mass Stream to				
- ~~Evaporize~~	**~~[kg/s]~~**	:		
- Condense	**[kg/s]**	:	n.a.	0.2768
Average Specific Heat	**[$kJ/kg \cdot ^oC$]**	:	4.18	-
Temperature IN	**[^oC]**	:	20.0	53.7
Temperature OUT	**[^oC]**	:	30.0	34.0
Pressure	**[bar]**	:	Atm.	0.15
Material *(5)*		:	n.a.	CS

Remarks:

(1) Heat capacity simulate from ASPEN

(2) Capacity = Area × Overall Heat Transfer Coefficient × LMTD

(3) $\Delta T_{lm} = \dfrac{(T_1 - t_2) - (T_2 - t_1)}{\ln \dfrac{(T_1 - t_2)}{(T_2 - t_1)}}$ [15] (p598 equation 12.4)

(4) [15] (p697, *for single tube heat exchanger typical effectiveness 1*)

(5) CS = Carbon Steel

Table A5.11.14: Equipment data specification sheet of product cooler E104

PRODUCT COOLER E104 – DATA SPECIFICATION SHEET

EQUIPMENT NUMBER	:	**E104**	**In Series**	:	1
NAME	:	***C101 Product cooler***	**In Parallel**	:	none

General Data

Service : - **Heat Exchanger(Water cooled)**
- ~~**Vaporizer**~~ - ~~**Condenser**~~
- ~~**Cooler**~~ - ~~**Reboiler**~~

Type : - ~~**Fixed Tube Sheets**~~ - ~~**Plate Heat Exchanger**~~
- ~~**Floating Head**~~ - ~~**Finned Tubes**~~
- ~~**Hair Pin**~~ - ~~**Thermosyphon**~~
- ~~**Double Tube**~~ - **Single Tube**

Position : - **Horizontal**
- ~~**Vertical**~~

Capacity	**[kW]**	:	1.55	*(1)*	**(Calc.)**
Heat Exchange Area	**[m^2]**	:	0.26	*(2)*	**(Calc.)**
Overall Heat Transfer Coefficient	**[W/m^2·^{o}C]**	:	250		**(Approx.)**
Log. Mean Temperature Diff. (LMTD)	**[^{o}C]**	:	24.19	*(3)*	
Passes Tube Side		:	1		
Passes Shell Side		:	1		
Correction Factor LMTD (min. 0.75)		:	1.0	*(4)*	
Corrected LMTD	**[^{o}C]**	:	24.19		

Process Conditions

			Shell Side	**Tube Side**
Medium		:	Cooling water	Toluene / Precursor
Mass Stream	**[kg/s]**	:	0.037	0.0177
Mass Stream to				
- ~~**Evaporize**~~	~~**[kg/s]**~~	:		
- **Condense**	**[kg/s]**	:	n.a.	0.0177
Average Specific Heat	**[kJ/kg·^{o}C]**	:	4.18	-
Temperature IN	**[^{o}C]**	:	20.0	98.2
Temperature OUT	**[^{o}C]**	:	30.0	25
Pressure	**[bar]**	:	Atm.	0.15
Material *(5)*		:	n.a.	CS

Remarks:

(1) Heat capacity simulate from ASPEN
(2) Capacity = Area × Overall Heat Transfer Coefficient × LMTD
(3) $\Delta T_{lm} = \dfrac{(T_1 - t_2) - (T_2 - t_1)}{\ln \dfrac{(T_1 - t_2)}{(T_2 - t_1)}}$ [15] (p598 equation 12.4)
(4) [15] (p697, *for single tube heat exchanger typical effectiveness 1)*
(5) CS = Carbon Steel

Table A5.11.15: Equipment data specification sheet of lipase B separation filter F101

FILTER F101 – DATA SPECIFICATION SHEET			
EQUIPMENT NUMBER: F101		**In Series :**	1
NAME	**: *Lipase B separation filter***	**In Parallel :**	none

Service : Lipase B separation filter
Type : Microfilter
Number : 1

Operating Conditions & Physical Data

Separation phases		**:**	Solid/Liquid
Exit temperature	**[^{0}C]**	**:**	30
Average filtrate flux	**[l/m^{2}h]**	**:**	20
Max. concentration of solid	**[g/liter]**	**:**	600
Filtration mode (**Batch concentration =1, Feed and bleed=2)**		**:**	1
For each component rejection coefficient		**:**	0

Cost

Unit power consumption	**[kW/m^2]**	**:**	0.2
Membrane replacement cost	**[operating hrs]**	**:**	2000
Unit membrane cost	**[$/m^2]**	**:**	200

Design Mode

Concentration factor(Feed/Retentate)		**:**	1
Max. Area	**[m^2]**	**:**	80

Rating Mode

Membrane Area	**[m^2]**	**:**	80
Number of units		**:**	1

Remarks:
- The filter chosen from SUPERPRO Design. Default design of Microfilter is used
- Design the max. membrane area as 80 m^2

Table A5.11.16: Equipment data specification sheet of lanthanum hydroxide separation filter F102

FILTER F102 – DATA SPECIFICATION SHEET			
EQUIPMENT NUMBER :	**F102**	**In Series :**	1
NAME :	***$La(OH)_3$ separation filter***	**In Parallel :**	none
Service : $La(OH)_3$ separation filter **Type :** Microfilter **Number :** 1			
Operating Conditions & Physical Data			
Separation phases		:	Solid/Liquid
Exit temperature	**[^{0}C]**	:	30
Average filtrate flux	**[l/m^2h]**	:	20
Max. concentration of solid	**[g/liter]**	:	600
Filtration mode **(Batch concentration =1, Feed and bleed=2)**		:	1
For each component rejection coefficient		:	0
Cost			
Unit power consumption	**[kw/m^2]**	:	0.2
Membrane replacement cost	**[operating hrs]**	:	2000
Unit membrane cost	**[$\$/m^2$]**	:	200
Design Mode			
Concentration factor(Feed/Retentate)		:	1
Max. Area	**[m^2]**	:	80
Rating Mode			
Membrane Area	**[m^2]**	:	80
Number of units		:	1
Remarks: - The filter chosen from SUPERPRO Design. Default design of Microfilter is used - Design the max. membrane area as 80 m^2			

Table A5.11.17: Equipment data specification sheet of toluene transport pump P101

PUMP P101 – DATA SPECIFICATION SHEET

EQUIPMENT NUMBER : **P101**		**Operating** :	1
NAME : ***Toluene Transport Pump***		**Installed Spare** :	1

Service : Toluene transfer pump
Type : Centrifugal
Number : 2

Operating Conditions & Physical Data

Pumped liquid:	Toluene			
Temperature	**(T)**	**[^{o}C]**	:	25.0
Density	**(ρ)**	**[kg/m^3]**	:	866
Viscosity	**(η)**	**[N·s/m^2]**	:	0.0001

Power

Capacity	**(Φ_v)**	**[m^3/s]**	:	0.001	
Suction Pressure	**(p_s)**	**[bar]**	:	0.939	
Discharge Pressure	**(p_d)**	**[bar]**	:	4.91	
Theoretical Power		**[kW]**	:	0.4	$\{ = \Phi_V \cdot (p_d - p_s) \cdot 10^2 \}$
Pump Efficiency		**[-]**	:	0.27	[15] (p435)
Power at Shaft		**[kW]**	:	1.5	

Construction Details *(1)*

RPM		:	3000	**Nominal diameter**		
Drive		:	Electrical	**Suction Nozzle**	**[…]**	:
Type electrical motor		:		**Discharge Nozzle**	**[…]**	:
Tension	**[V]**	:	380	**Cooled Bearings**		: **Yes / No**
Rotational direction		:	**Clock /** ~~**Counter Cl.**~~	**Cooled Stuffing Box**		: **Yes / No**
				Smothering Gland		: **Yes / No**
Foundation Plate		:	**Combined /** ~~**two parts**~~	**If yes**		
				- Seal Liquid		: **Yes / No**
Flexible Coupling		:	Yes	**- Splash Rings**		: **Yes / No**
Pressure Gauge Suction		:	No	**- Packing Type**		:
Pressure Gauge Discharge		:	Yes	**- Mechanical Seal**		: **Yes / No**
Min. Overpressure above				**- N.P.S.H. [m]**		:
p_v/p_m	**[bar]**	:	0.1	**$\{ = p_m \cdot \rho \cdot g \}$**		

Construction Materials *(2)*

Pump House		:	MS	**Wear Rings**		:
Pump Rotor		:	HT Steel	**Shaft Box**		:
Shaft		:	HT Steel			
Special provisions		:	none			
Operating Pressure	**[bar]**	:	2	**Test Pressure**	**[bar]**	:

Remarks:
(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist
(2) MS = Mild Steel; HT Steel = High Tensile Steel

Table A5.11.18: Equipment data specification sheet of liquid transport pump P102

PUMP P102 – DATA SPECIFICATION SHEET

EQUIPMENT NUMBER	:	**P102**	**Operating**	: 1
NAME	:	***Liquid Transport Pump***	**Installed Spare**	: 1

Service	:	Liquid transfer pump
Type	:	Centrifugal
Number	:	2

Operating Conditions & Physical Data

Pumped liquid:	Catalyst (lanthanum isopropoxide) dissolved in toluene			
Temperature	**(T)**	**[^oC]**	:	25.0
Density	**(ρ)**	**[kg/m^3]**	:	873.6
Viscosity	**(η)**	**[$N \cdot s/m^2$]**	:	0.0001

Power

Capacity	**(Φ_v)**	**[m^3/s]**	:	0.002	
Suction Pressure	**(p_s)**	**[bar]**	:	0.937	
Discharge Pressure	**(p_d)**	**[bar]**	:	3.594	
Theoretical Power		**[kW]**	:	0.52	$\{ = \Phi_V \cdot (p_d - p_s) \cdot 10^2 \}$
Pump Efficiency		**[-]**	:	0.42	[15] (p435)
Power at Shaft		**[kW]**	:	1.3	

Construction Details *(1)*

RPM		:	3000	**Nominal diameter**			
Drive		:	Electrical	**Suction Nozzle**	**[…]**	:	
Type electrical motor		:		**Discharge Nozzle**	**[…]**	:	
Tension	**[V]**	:	380	**Cooled Bearings**		:	**Yes / No**
Rotational direction		:	**Clock / ~~Counter Cl.~~**	**Cooled Stuffing Box**		:	**Yes / No**
				Smothering Gland		:	**Yes / No**
Foundation Plate		:	**Combined / ~~two parts~~**	**If yes**			
				- Seal Liquid		:	**Yes / No**
Flexible Coupling		:	Yes	**- Splash Rings**		:	**Yes / No**
Pressure Gauge Suction		:	No	**- Packing Type**		:	
Pressure Gauge Discharge		:	Yes	**- Mechanical Seal**		:	**Yes / No**
Min. Overpressure above				**- N.P.S.H.**	**[m]**	:	
p_v/p_m	**[bar]**	:	0.1	**$\{ = p_m \cdot \rho \cdot g \}$**			

Construction Materials *(2)*

Pump House		:	MS	**Wear Rings**		:	
Pump Rotor		:	HT Steel	**Shaft Box**		:	
Shaft		:	HT Steel				
Special provisions		:	none				
Operating Pressure	**[bar]**	:	2	**Test Pressure**	**[bar]**	:	

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) MS = Mild Steel; HT Steel = High Tensile Steel

Table A5.11.19: Equipment data specification sheet of liquid transport pump P103

PUMP P103 – DATA SPECIFICATION SHEET							
EQUIPMENT NUMBER	**:**	**P103**		**Operating**		**:**	1
NAME	**:**	***Liquid Transport Pump***		**Installed Spare**		**:**	1
Service	**:**	Liquid transfer pump					
Type	**:**	Centrifugal					
Number	**:**	2					
Operating Conditions & Physical Data							
Pumped liquid:	Reaction mixture						
Temperature	**(*T*)**	**[°C]**	**:**	25.0			
Density	**(ρ)**	**[kg/m^3]**	**:**	904.5			
Viscosity	**(η)**	**[N·s/m^2]**	**:**	0.0001			
Power							
Capacity	**(Φ_v)**	**[m^3/s]**	**:**	0.000553			
Suction Pressure	**(p_s)**	**[bar]**	**:**	0.908			
Discharge Pressure	**(p_d)**	**[bar]**	**:**	3.708			
Theoretical Power		**[kW]**	**:**	0.15	$\{ = \Phi_V \cdot (p_d - p_s) \cdot 10^2 \}$		
Pump Efficiency		**[-]**	**:**	0.23	[15] (p435)		
Power at Shaft		**[kW]**	**:**	0.7			
Construction Details *(1)*							
RPM		**:**	3000	**Nominal diameter**			
Drive		**:**	Electrical	**Suction Nozzle**	**[…]**	**:**	
Type electrical motor		**:**		**Discharge Nozzle**	**[…]**	**:**	
Tension	**[V]**	**:**	380	**Cooled Bearings**		**:**	**Yes / No**
Rotational direction		**:**	**Clock / ~~Counter Cl.~~**	**Cooled Stuffing Box**		**:**	**Yes / No**
				Smothering Gland		**:**	**Yes / No**
Foundation Plate		**:**	**Combined / ~~two parts~~**	**If yes**			
				- Seal Liquid		**:**	**Yes / No**
Flexible Coupling		**:**	Yes	**- Splash Rings**		**:**	**Yes / No**
Pressure Gauge Suction		**:**	No	**- Packing Type**		**:**	
Pressure Gauge Discharge		**:**	Yes	**- Mechanical Seal**		**:**	**Yes / No**
Min. Overpressure above				**- N.P.S.H.**	**[m]**	**:**	
p_v/p_m	**[bar]**	**:**	0.1	$\{ = p_m \cdot \rho \cdot g \}$			
Construction Materials *(2)*							
Pump House		**:**	MS	**Wear Rings**		**:**	
Pump Rotor		**:**	HT Steel	**Shaft Box**		**:**	
Shaft		**:**	HT Steel				
Special provisions		**:**	none				
Operating Pressure	**[bar]**	**:**	2	**Test Pressure**	**[bar]**	**:**	

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) MS = Mild Steel; HT Steel = High Tensile Steel

Table A5.11.20: Equipment data specification sheet of distillation column's feed pump P104

PUMP P104 – DTA SPECIFICATION SHEET						
EQUIPMENT NUMBER :	**P104**			**Operating**	**:**	1
NAME :	***C101 feed Pump***			**Installed Spare**	**:**	1
Service :	Column feed pump					
Type :	Centrifugal					
Number :	2					
Operating Conditions & Physical Data						
Pumped liquid:	Reaction mixture					
Temperature	**(T)**	**[^oC]**	**:**	25.0		
Density	**(ρ)**	**[kg/m^3]**	**:**	897		
Viscosity	**(η)**	**[$N \cdot s/m^2$]**	**:**	0.0001		
Power						
Capacity	**(Φ_v)**	**[m^3/s]**	**:**	0.000236		
Suction Pressure	**(p_s)**	**[bar]**	**:**	0.842		
Discharge Pressure	**(p_d)**	**[bar]**	**:**	5.195		
Theoretical Power		**[kW]**	**:**	0.11	$\{ = \Phi_V \cdot (p_d - p_s) \cdot 10^2 \}$	
Pump Efficiency		**[-]**	**:**	0.17	[15] (p435)	
Power at Shaft		**[kW]**	**:**	0.7		

Construction Details *(1)*

RPM		**:**	3000	**Nominal diameter**			
Drive		**:**	Electrical	**Suction Nozzle**	**[…]**	**:**	
Type electrical motor		**:**		**Discharge Nozzle**	**[…]**	**:**	
Tension	**[V]**	**:**	380	**Cooled Bearings**		**:**	**Yes / No**
Rotational direction		**:**	**Clock / ~~Counter Cl.~~**	**Cooled Stuffing Box**		**:**	**Yes / No**
				Smothering Gland		**:**	**Yes / No**
Foundation Plate		**:**	**Combined / ~~two parts~~**	**If yes**			
				- Seal Liquid		**:**	**Yes / No**
Flexible Coupling		**:**	Yes	**- Splash Rings**		**:**	**Yes / No**
Pressure Gauge Suction		**:**	No	**- Packing Type**		**:**	
Pressure Gauge Discharge		**:**	Yes	**- Mechanical Seal**		**:**	**Yes / No**
Min. Overpressure above p_v/p_m	**[bar]**	**:**	0.1	**- N.P.S.H.** $\{ = p_m \cdot \rho \cdot g \}$	**[m]**	**:**	

Construction Materials *(2)*

Pump House		**:**	MS	**Wear Rings**		**:**
Pump Rotor		**:**	HT Steel	**Shaft Box**		**:**
Shaft		**:**	HT Steel			
Special provisions		**:**	none			
Operating Pressure	**[bar]**	**:**	3	**Test Pressure**	**[bar]**	**:**

Remarks:
(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.
(2) MS = Mild Steel; HT Steel = High Tensile Steel

Table A5.11.21: Equipment data specification sheet of vacuum pump P105

PUMP P105 – DATA SPECIFICATION SHEET						
EQUIPMENT NUMBER		**:**	**P105**	**Operating**	**:**	1
NAME		**:**	***Vacuum Pump***	**Installed Spare**	**:**	1
Service		**:**	create vacuum			
Type		**:**	rotary			
Number		**:**	2			
Operating Conditions & Physical Data						
Pumped medium:	air					
Temperature	**(T)**	**[^{o}C]** **:**	20.0			
Density	**(ρ)**	**[kg/m^3]** **:**	1.2			
Viscosity	**(η)**	**[N·s/m^2]** **:**	0.00002			
Vapour Pressure	**(p_v)**	**[bar]** **:**	0.15-1.0	**at Temperature [^{o}C]**	**:**	20.0
Power						
Capacity	**(Φ_v)**	**[m^3/s]** **:**	0.008			
Suction Pressure	**(p_s)**	**[bar]** **:**	0.144			
Discharge Pressure	**(p_d)**	**[bar]** **:**	3.265			
Theoretical Power		**[kW]** **:**	2.5	**{ = $\Phi_v \cdot (p_d - p_s) \cdot 10^2$ }**		
Pump Efficiency		**[-]** **:**	0.9			
Power at Shaft		**[kW]** **:**	2.8			
Construction Details *(1)*						
RPM		**:**		**Nominal diameter**		
Drive		**:**	Electrical	**Suction Nozzle** **[…]**	**:**	
Type electrical motor		**:**		**Discharge Nozzle** **[…]**	**:**	
Tension	**[V]**	**:**	380	**Cooled Bearings**	**:**	**Yes / No**
Rotational direction		**:**	**Clock / ~~Counter Cl.~~**	**Cooled Stuffing Box**	**:**	**Yes / No**
				Smothering Gland	**:**	**Yes / No**
Foundation Plate		**:**	**Combined / ~~two parts~~**	**If yes**		
				- Seal Liquid	**:**	**Yes / No**
Flexible Coupling		**:**	Yes	**- Splash Rings**	**:**	**Yes / No**
Pressure Gauge Suction		**:**	No	**- Packing Type**	**:**	
Pressure Gauge Discharge		**:**	Yes	**- Mechanical Seal**	**:**	**Yes / No**
Min. Overpressure above				**- N.P.S.H.** **[m]**	**:**	
p_v/p_m	**[bar]**	**:**	0.1	**{ = $p_m \cdot \rho \cdot g$ }**		
Construction Materials *(2)*						
Pump House		**:**	MS	**Wear Rings**	**:**	
Pump Rotor		**:**	HT Steel	**Shaft Box**	**:**	
Shaft		**:**	HT Steel			
Special provisions		**:**	none			
Operating Pressure	**[bar]**	**:**	0.15bar	**Test Pressure** **[bar]**	**:**	

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) MS = Mild Steel; HT Steel = High Tensile Steel

Table A5.11.22: Equipment data specification sheet of reflux pump P106

PUMP P106 – DATA SPECIFICATION SHEET

EQUIPMENT NUMBER	**:**	**P106**	**Operating**	**:**	1
NAME	**:**	***Toluene Reflux Pump***	**Installed Spare**	**:**	1

Service : Toluene reflux
Type : centrifugal
Number : 2

Operating Conditions & Physical Data

Pumped liquid:	Toluene/Product				
Temperature	**(T)**	**[°C]**	: 34.0		
Density	**(ρ)**	**[kg/m^3]**	: 854.7		
Viscosity	**(η)**	**[N·s/m^2]**	: 0.0001		
Vapour Pressure	**(p_v)**	**[bara] :**	0.15	**at Temperature [°C] :**	34.0

Power

Capacity	**(Φ_v)**	**[m^3/s]**	:	1×10^{-4}	
Suction Pressure	**(p_s)**	**[bar]**	:	0.297	
Discharge Pressure	**(p_d)**	**[bar]**	:	2.359	
Theoretical Power		**[kW]**	:	0.021	**{ = $\Phi_v \cdot (p_d - p_s) \cdot 10^2$ }**
Pump Efficiency		**[-]**	:	0.2	
Power at Shaft		**[kW]**	:	0.11	

Construction Details *(1)*

RPM		:		**Nominal diameter**			
Drive		:	Electrical	**Suction Nozzle**	**[…]**	:	
Type electrical motor		:		**Discharge Nozzle**	**[…]**	:	
Tension	**[V]**	:	380	**Cooled Bearings**		:	**Yes / No**
Rotational direction		:	**Clock / ~~Counter Cl.~~**	**Cooled Stuffing Box**		:	**Yes / No**
				Smothering Gland		:	**Yes / No**
Foundation Plate		:	**Combined / ~~two parts~~**	**If yes**			
				- Seal Liquid		:	**Yes / No**
Flexible Coupling		:	Yes	**- Splash Rings**		:	**Yes / No**
Pressure Gauge Suction		:	No	**- Packing Type**		:	
Pressure Gauge Discharge		:	Yes	**- Mechanical Seal**		:	**Yes / No**
Min. Overpressure above				**- N.P.S.H.**	**[m]**	:	
p_v/p_m	**[bar]**	:	0.1	**{ = $p_m \cdot \rho \cdot g$ }**			

Construction Materials *(2)*

Pump House		:	MS	**Wear Rings**		:
Pump Rotor		:	HT Steel	**Shaft Box**		:
Shaft		:	HT Steel			
Special provisions		:	none			
Operating Pressure	**[bar]**	:	0.15bar	**Test Pressure**	**[bar]**	:

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) MS = Mild Steel; HT Steel = High Tensile Steel

Table A5.11.23: Equipment data specification sheet of toluene transport pump P107

PUMP P107 – DATA SPECIFICATION SHEET							
EQUIPMENT NUMBER :	**P107**			**Operating**		:	1
NAME :	***Toluene Transfer Pump***			**Installed Spare**		:	1
Service :	Toluene transfer						
Type :	centrifugal						
Number :	2						
Operating Conditions & Physical Data							
Pumped liquid:	Technical grade toluene						
Temperature	**(T)**	**[^oC]**	: 34.0				
Density	**(ρ)**	**[kg/m^3]**	: 854.7				
Viscosity	**(η)**	**[$N{\cdot}s/m^2$]**	: 0.0001				
Vapour Pressure	**(p_v)**	**[bar]** :	0.15	**at Temperature [^oC] :**			34.0
Power							
Capacity	**(Φ_v)**	**[m^3/s]** :	2.2×10^{-4}				
Suction Pressure	**(p_s)**	**[bar]** :	0.201				
Discharge Pressure	**(p_d)**	**[bar]** :	3.99				
Theoretical Power		**[kW]** :	0.09	$\{ = \Phi_v \cdot (p_d - p_s) \cdot 10^2 \}$			
Pump Efficiency		**[-]** :	0.2				
Power at Shaft		**[kW]** :	0.45				
Construction Details *(1)*							
RPM		:		**Nominal diameter**			
Drive		:	Electrical	**Suction Nozzle**	**[…]**	:	
Type electrical motor		:		**Discharge Nozzle**	**[…]**	:	
Tension	**[V]**	:	380	**Cooled Bearings**		:	**Yes / No**
Rotational direction		:	**Clock / ~~Counter Cl.~~**	**Cooled Stuffing Box**		:	**Yes / No**
				Smothering Gland		:	**Yes / No**
Foundation Plate		:	**Combined / ~~two parts~~**	**If yes**			
				- Seal Liquid		:	**Yes / No**
Flexible Coupling		:	Yes	**- Splash Rings**		:	**Yes / No**
Pressure Gauge Suction		:	No	**- Packing Type**		:	
Pressure Gauge Discharge		:	Yes	**- Mechanical Seal**		:	**Yes / No**
Min. Overpressure above				**- N.P.S.H.**	**[m]**	:	
p_v/p_m	**[bar]**	:	0.1	$\{ = p_m \cdot \rho \cdot g \}$			
Construction Materials *(2)*							
Pump House		:	MS	**Wear Rings**		:	
Pump Rotor		:	HT Steel	**Shaft Box**		:	
Shaft		:	HT Steel				
Special provisions		:	none				
Operating Pressure	**[bar]**	:	0.15bar	**Test Pressure**	**[bar]**	:	

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) (2) MS = Mild Steel; HT Steel = High Tensile Steel

Table A5.11.24: Equipment data specification sheet of product transport pump P108

PUMP P108 – DATA SPECIFICATION SHEET

EQUIPMENT NUMBER	**:**	**P 108**	**Operating**	**:**	1
NAME	**:**	***Product Transfer Pump***	**Installed Spare**	**:**	1

Service **:** Product transfer
Type **:** diaphragm
Number **:** 2

Operating Conditions & Physical Data

Pumped liquid:	Product (precursor of Prozac)					
Temperature	**(T)**	**[^oC]**	**:**	100.0		
Density	**(ρ)**	**[kg/m^3]**	**:**	1202.8		
Viscosity	**(η)**	**[$N{\cdot}s/m^2$]**	**:**	0.0003		
Vapour Pressure	**(p_v)**	**[bar]**	**:**	0.15	**at Temperature [^oC] :**	100.0

Power

Capacity	**(Φ_v)**	**[m^3/s]**	**:**	1.5×10^{-5}	
Suction Pressure	**(p_s)**	**[bar]**	**:**	0.60	
Discharge Pressure	**(p_d)**	**[bar]**	**:**	4.80	
Theoretical Power		**[kW]**	**:**	0.0063	**$\{ = \Phi_V \cdot (p_d - p_s) \cdot 10^2 \}$**
Pump Efficiency		**[-]**	**:**	0.5	
Power at Shaft		**[kW]**	**:**	0.013	

Construction Details *(1)*

RPM		**:**		**Nominal diameter**				
Drive		**:**		**Suction Nozzle**	**[…]**	**:**		
Type electrical motor		**:**		**Discharge Nozzle**	**[…]**	**:**		
Tension	**[V]**	**:**		**Cooled Bearings**		**:**	**Yes / No**	
Rotational direction		**:**	**Clock / ~~Counter Cl.~~**	**Cooled Stuffing Box**		**:**	**Yes / No**	
				Smothering Gland		**:**	**Yes / No**	
Foundation Plate		**:**	**Combined / ~~two parts~~**	**If yes**				
				- Seal Liquid		**:**	**Yes / No**	
Flexible Coupling		**:**	Yes	**- Splash Rings**		**:**	**Yes / No**	
Pressure Gauge Suction		**:**	No	**- Packing Type**		**:**		
Pressure Gauge Discharge		**:**	Yes	**- Mechanical Seal**		**:**	**Yes / No**	
Min. Overpressure above				**- N.P.S.H.**	**[m]**	**:**		
p_v/p_m	**[bar]**	**:**	0.1	**$\{ = p_m \cdot \rho \cdot g \}$**				

Construction Materials *(2)*

Pump House		**:**	MS	**Wear Rings**		**:**	
Pump Rotor		**:**	HT Steel	**Shaft Box**		**:**	
Shaft		**:**	HT Steel				
Special provisions		**:**	none				
Operating Pressure	**[bar]**	**:**	0.15bar	**Test Pressure**	**[bar]**	**:**	

Remarks:

(1) Double mechanical seals and seal fluid required for LPG service. Further details to be specified by Rotating Equipment specialist.

(2) MS = Mild Steel; HT Steel = High Tensile Steel

A5.2 Design of dissolving tank T102

A5.2.1 Dimensioning of the dissolving tank

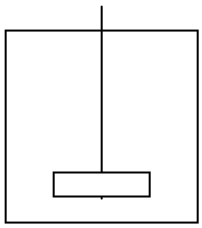
Table A5.2.1: The volume of the components in dissolving tank T102

Components	*Density (kg/l)*	*Weight (kg)*	*Volume (l)*	*Volume (m^3)*
Toluene	0.866	520.12		
Lanthanum isopropoxide	4.4	5.70		
Total		525.82	601.9	0.602
Average	0.873602			

The volume of the mixture is 0.602m^3. It is designed that the liquid only occupies 80% of the volume of the tank (for safety reason), so the total design volume of the reactor is 0.7525m^3.

The diameter of the tank is chosen to be 1m and by using the following equation $V = \frac{\pi}{4} D^2 H$, the height of tank is calculated to be 0.96m.

A5.2.2 Design of the stirrer and mixing time calculation



$$N_{mix} = \frac{t_m \varepsilon^{1/3}}{D^{2/3}} = \frac{\alpha}{\beta^{4/3}\gamma^{1/3}} \left(\frac{L_s}{H}\right)^2 \left(\frac{H}{D}\right)^2 \quad \text{[14]} \qquad (1)$$

where:

N_{mix}	Mixing number	
t_m	Mixing time	[s]
ε	Total specific power input	[W/kg]
D	Diameter of reactor	[m]
α	Homogeneity factor	Using a homogeneity of 95% and maximum distance α =0.374
β	Primary eddy size	$\beta = \frac{H_s}{D}$ (H_s is blade height)
γ	Average viscosity index	34.16
L_s	Flow path length	[m]
H	Reactor height	[m]

L_S = H + 2D = 0.96D + 2D = 2.96D

$$\frac{L_S}{H} = \frac{2.96D}{0.96D} = 3.08 \ ;$$

$$\varepsilon = \frac{P_S}{\rho_L V} = \frac{N_I \frac{1}{2} c\pi^4 \rho_L N^3 D'^5}{\rho_L \pi \frac{D^2}{4} H} = \frac{N_I N_P N^3 D'^5}{\pi \frac{D^2}{4} H} \quad \text{[14]} \qquad (2)$$

$$c = \frac{H_S}{D'} \qquad (3)$$

where:

P_s	Power input per stirrer	[W]
ρ_L	Density for the liquid	[kg/m^3]
V	Reactor volume	[m^3]
D'	Stirrer diameter	[m] D'=1/3D assume it is Rushton stirrer.
D	Reactor diameter	[m]
c	Ratio	
N_p	Power number	6 (Rushton)
N	Angle speed	

$$\frac{1}{2}c\pi^4 = N_P \to c = \frac{2N_P}{\pi^4} = \frac{2\times 6}{\pi^4} = 0.123$$

$$H_S = cD' = 0.123D' \to D' = 8H_S$$

$$\beta = \frac{H_S}{D} = \frac{H_S}{3D'} = \frac{H_S}{3\times 8H_S} = \frac{1}{24} = 0.0416$$

$$N_{mix} = \frac{\alpha}{\beta^{4/3}\gamma^{1/3}}\left(\frac{L_s}{H}\right)^2\left(\frac{H}{T}\right) = \frac{0.374}{(0.0416)^{4/3}(34.16)^{1/3}}(3.08)^2(0.96)^2 = 70.0619$$

From equation (1): $N_{mix} = \dfrac{t_m \varepsilon^{1/3}}{D^{2/3}} \to t_m = \dfrac{N_{mix}D^{2/3}}{\varepsilon^{1/3}}$ (4)

From calculation in A5.2.1: V = 0.7525m^3 and D = 1m, hence:

$$t_m = \frac{N_{mix}D^{2/3}}{\varepsilon^{1/3}} = \frac{70.0619\times(1)^{2/3}}{\varepsilon^{1/3}}$$

Because the low power input (suspending light solids, blending low-viscosity liquid) for stirred tank is 0.2kW/m^3 [20] therefore, for the dissolving tank T102 (V = 0.7525m^3) the power needs to be input is P_s = 0.2kW/m^3 × 0.7525m^3 = 0.1505kW

Total specific power ε is can be determined from the formula: $\varepsilon = \dfrac{Power\ P_s(W)}{Mass(kg)}$, which is 150.5W/525.817kg = 0.2862W/kg.

Using equation (4) the mixing time is calculated to be 106.3s.

Because the dissolving process is very fast, so the operation time is decided to be 10 minutes to make sure all the catalyst (lanthanum isopropoxide) is dissolved in toluene. By choosing the operation time of 10mins (600s), the mixing time of 106s calculated above is also acceptable.

A5.3 Design of batch reactor R101

A5.3.1 Dimensioning of the reactor

Table A5.3.1: The volume of the liquid in reactor R101

Component	*Input (kg/batch)*	*Density (kg/l)*	*Volume (m^3)*	*Remarks*
Propenyl Acetate	36.08	0.909	0.0397	(1) refer to part 5.4, chapter 5 for the input per batch (2) refer to part 3.2.4, chapter 3 for the density of the components
Toluene	520.12	0.866	0.6006	
(R)-3-chloro-1-phenylpropyl acetate	40.96	1.5412	0.0266	
Total			0.6669	

The volume of the mixture is 0.6669m^3. It is designed that the liquid only occupies 80% of the volume of the reactor (for safety reason), so the total design volume of the reactor is 0.8336m^3.

Diameter and height chosen:

The following formulas are used to calculated the diameter, height and heat exchange area of the reactor:

$$V = \frac{\pi}{4} D^2 H \qquad V_{liquid} = \frac{\pi}{4} D^2 H_{liquid} \qquad A = \pi D H$$

$$\frac{V}{A} = \frac{D}{4} \qquad D = \frac{4V}{A} \qquad A_{useful} = \pi D H_{liquid}$$

Table A5.3.2: Comparison of the heat exchange area for the decision on the dimensions of the reactor

Diameter (m)	*Height (m)*	*Heat exchange area (m^2)*	*Liquid height (m)*	*Useful heat exchange area (m^2)*
0.5	4.2454	6.6686	3.3963	5.3349
0.6	2.9482	5.5572	2.3585	4.4458
0.7	2.1660	4.7633	1.7328	3.8107
0.8	1.6584	4.1679	1.3267	3.3343
0.9	1.3103	3.7048	1.0482	2.9638
1	1.0613	3.3343	0.8491	2.6675

N.B. Because the diameter for normal reactor is always less than 1 m, so longer diameters were not considered in the table above.

The smallest heat exchange area is chosen because it leads to lower cost for construction of reactor.

Therefore the dimension of the reactor is: diameter D = 1m, height H = 1.07m.

A5.3.2 Design of the stirrer and mixing time calculation

$$N_{mix} = \frac{t_m \varepsilon^{1/3}}{D^{2/3}} = \frac{\alpha}{\beta^{4/3}\gamma^{1/3}}\left(\frac{L_s}{H}\right)^2\left(\frac{H}{D}\right)^2 \quad [14] \qquad (1)$$

N_{mix}	Mixing Number	
t_m	Mixing time	[s]
ε	Total specific power input	[W/kg]
D	Diameter of reactor	[m]
α	Homogeneity factor	Using a homogeneity of 95% and maximum distance α =0.374
β	Primary eddy size	$\beta = \frac{H_s}{D}$ (H_s is blade height)
γ	Average viscosity index	35.013
L_s	Flow path length	[m]
H	Reactor height	[m]

L_S = H + 2D = 1.07D + 2D = 3.07D

$$\frac{L_S}{H} = \frac{3.07D}{1.07D} = 2.87\,;$$

$$\varepsilon = \frac{P_S}{\rho_L V} = \frac{N_I \frac{1}{2} c\pi^4 \rho_L N^3 D'^5}{\rho_L \pi \frac{D^2}{4} H} = \frac{N_I N_P N^3 D'^5}{\pi \frac{D^2}{4} H} \qquad (2)$$

$$c = \frac{H_S}{D'} \qquad (3)$$

P_s	Power input per stirrer	[W]
ρ_L	Density for the liquid	[kg/m^3]
V	Reactor volume	[m^3]
D’	Stirrer diameter	[m] D’=1/3D assume it is Rushton stirrer.
D	Reactor diameter	[m]
c	Ratio	
N_p	Power number	6 (Rushton)
N	Angle speed	

$$\frac{1}{2}c\pi^4 = N_P \rightarrow c = \frac{2N_P}{\pi^4} = \frac{2\times 6}{\pi^4} = 0.123 \quad [14] \qquad (4)$$

$$H_S = cD' = 0.123D' \rightarrow D' = 8H_S \quad [14] \qquad (5)$$

$$\beta = \frac{H_S}{D} = \frac{H_S}{3D'} = \frac{H_S}{3\times 8H_S} = \frac{1}{24} = 0.0416$$

$$N_{mix} = \frac{\alpha}{\beta^{4/3}\gamma^{1/3}}\left(\frac{L_s}{H}\right)^2\left(\frac{H}{T}\right) = \frac{0.374}{(0.0416)^{4/3}(35.013)^{1/3}}(2.87)^2(1.07)^2 = 74.79434$$

From equation (1): $N_{mix} = \dfrac{t_m \varepsilon^{1/3}}{D^{2/3}} \rightarrow t_m = \dfrac{N_{mix} D^{2/3}}{\varepsilon^{1/3}}$ (6)

From calculation in A5.3.1: V = 0.84m^3 and D = 1m, hence:

$$t_m = \frac{N_{mix} D^{2/3}}{\varepsilon^{1/3}} = \frac{74.79434 \times (1)^{2/3}}{\varepsilon^{1/3}}$$

Because the low power input (suspending light solids, blending low-viscosity liquid) for stirred tank is 0.2kW/m^3 [20] therefore, for the reactor R101 (V = 0.84m^3) the power needs to be input is P_s = 0.2kW/m^3 × 0.84m^3 = 0.168kW

Total specific power ε is can be determined from the formula: $\varepsilon = \dfrac{Power\ P_s(W)}{Mass(kg)}$,

which is 168W/611.7kg = 0.275W/kg
(refer to part 5.4, chapter 5 for the mass per batch in the reactor)

Using equation (6) the mixing time is calculated to be 115 seconds

Because the heating time is 12.72 minutes (763.2s) (refer to appendix A4.3.1), so the mixing time of 115 seconds (during heating) is acceptable.

Stirrer diameter is calculated from the formula D' = D/3, in which D is reactor diameter, hence D' = 0.333m.

Stirrer height is calculated from equation (5), H_s = 0.041m

A5.4 Design of buffer tanks V101 and V103

A5.4.1 Buffer tank V101

(The buffer tank between filter F101 and precipitation tank T103)

The average filtrate flux through filter F101 is: $20\ l/m^2h \times 80m^2 = 1600l/h = 1.6m^3/h$ (refer to table A5.11.6, appendix A5.11)

Total liquid volume in the reactor is $0.6669m^3$ (refer to table A5.3.1, appendix A5.3), which is equal to the volume of the liquid passing through the filter

→ So the time needed for filtration is $0.6669\ m^3 / 1.6m^3h^{-1} = 0.4168h$ or 25min.

To transfer $0.6669m^3$ of liquid to precipitation tank it requires 20 min (refer to appendix A5.9.3 for pump P103 design) so the time difference between two processes is 5 min. It means that after 5min of filtration process, liquid from buffer tank can be pumped to precipitation tank. However, it is designed that after 10 minutes of the filtration process, pumping liquid from buffer tank to precipitation tank will start. After that these 2 processes will run at the same time, hence the filtration process will finish 5 minutes before the pumping process.

Therefore, the buffer tank should be designed big enough to contain the amount of liquid from the filter in first 10 minutes of the filtration process, which is:

$0.6669 \times 10/25 = 0.2668m^3$.

Because the filtrate flux in first several minutes always faster than average filtrate flux, so the volume f the buffer tank is designed 1.5 times more than the volume needed as calculated above. Hence the design volume of buffer tank V101 is:
$1.5 \times 0.2668 = 0.4m^3$

The diameter is designed to be 0.6m, and by using the following equation $V = \frac{\pi}{4} D^2 H$, the height of tank is calculated to be 1.45m.

A5.4.2 Buffer tank V103 in separation part

Table A5.4.1: The flow to the buffer tank V103

Component	*Flow to V103* (kg/h)	*Density* (kg/l)	*Flow* (l/h)	*Remarks*
Toluene	942.57	0.866	1088.42	(1) refer to table A4.2.1, appendix A4.5.2 for the flow to V103 (stream 25) (2) refer to table 3.2, part 3.2.4 for the density of the components
La-Isopropoxide	-			
R-, S- 3-chloro-1-phenyl-1-propanol	0	1.5412	0	
Lipase B	-			
Propenyl acetate	21.84	0.909	24.03	
(R)-3-chloro-1-phenylpropyl acetate	0.31	1.5121	0.20	
Acetone	25.27	0.7908	31.95	
Water	0.88	1	0.88	
Lanthanum Hydroxide				
Isopropanol	5.89	0.785	7.50	
Total			1152.99	

Buffer tank V103 is designed to accommodate the amount of liquid, which comes out from distillation column after 60 minutes of operation.

The volume of the liquid, which comes out from distillation column after 60 minutes (1h) of operation is 1153 litres (table A5.4.1) or 1.153 m^3

It is designed that the liquid only occupies 80% of the volume of the tank (for safety reason), so the total design volume is 1.441 m^3.

The diameter of the tank is chosen to be 1m and by using the following equation $V = \frac{\pi}{4} D^2 H$, the height of tank is calculated to be 1.84m.

A5.5 Design of precipitation tank T103

A5.5.1 Dimensioning of the reactor

Table A5.5.1: The volume of the liquid in precipitation tank T103

Component	*Quantity (kg/batch)*	*Density (kg/l)*	*Volume (l)*	*Remarks*
Propenyl acetate	12.050	0.909	13.257	(1) refer to table 5.2, chapter 5 for the quantity of each component (feed to T103, streams 15/16, and 17) (2) refer to part 3.2.4, chapter 3 for the density of the components
(R)-3-chloro-1-phenyl-1-propanol	0.041	1.5412	0.027	
Acetone	13.940	0.7908	17.627	
Toluene	520.12	0.866	600.600	
(R)-3-chloro-1-phenylpropyl acetate	51.000	1.5121	33.728	
Isopropanol	3.250	0.785	4.140	
Water	1.460	1.0	1.460	
Total			670.838	

The total volume of liquid in the precipitation tank is 670.838 litres or 0.6708 m^3.
It is designed that the liquid only occupies 80% of the volume of the tank (for safety reason), so the total design volume of the tank is 0.8385m^3.

The diameter of the tank is chosen to be 1m and by using the following equation $V = \frac{\pi}{4} D^2 H$, the height of tank is calculated to be 1.07m.

A5.5.2 Design of the stirrer and mixing time calculation

The size and the density of the liquid of the precipitation tank are the same as that of the reactor. Therefore, similar stirrers are designed for both of these equipments.

The stirrer diameter is 0.333m and the stirrer height is 0.041m. The mixing time is found to be 115s (refer to appendix A5.3 of reactor design for the same calculation approach).

The precipitation reaction is very fast [6], so the precipitation time is chosen to be 10 minutes to make sure all catalyst is precipitated. By choosing the operation time of 10mins (600s), the mixing time of 115s calculated above is also acceptable.

Because the low power input (suspending light solids, blending low-viscosity liquid) for stirred tank is 0.2kW/m^3 [20] therefore, for the precipitation tank T103 (V = 0.84m^3) the power needs to be input is P_s = 0.2kW/m^3 × 0.84m^3 = 0.168kW

A5.6 Design of intermediate storage tank V102

V102 is designed as intermediate storage tank, which can contains the liquid of reaction mixture of 20 batches coming from T103 (refer to part 8.2, chapter 8). The reason for choosing 20 batches is for designing good batch reactor size (please refer to part 2.2, chapter 2 for more explanation).

Table A5.6.1: The volume of the liquid in intermediate storage tank V102

Component	*Quantity feed to V102 after each batch (kg/batch)*	*Quantity in V102 $\times$ 20 batches (kg)*	*Density (kg/l)*	*Volume (l)*	*Remarks*
Propenyl acetate	12.050	241.0	0.909	265.14	(1) refer to table 5.2 chapter 5 for the quantity of each component (feed to V102, stream 20) (2) refer to part 3.2.4, chapter 3 for the density of the components
(R)-3-chloro-1-phenyl-1-propanol	0.041	0.82	1.5412	0.54	
Acetone	13.940	278.8	0.7908	352.55	
Toluene	520.12	10,402.4	0.866	12,012.0	
(R)-3-chloro-1-phenylpropyl acetate	51.000	1020.0	1.5121	674.56	
Isopropanol	3.250	65.0	0.785	82.80	
Water	0.487	9.74	1.0	9.74	
Total				13,397.3	

The total volume of liquid in intermediate storage tank is 13,397 litres or 13.4 m^3.
It is designed that the liquid only occupies 80% of the volume of the tank (for safety reason), so the total design volume of the tank is 16.75m^3.

The diameter of the tank is chosen to be 2.5m and by using the following equation $V = \frac{\pi}{4} D^2 H$, the height of tank is calculated to be 3.5m.

A5.7 Design of distillation column C101

In this appendix A5.7, dimensioning of the distillation column is explained according to the Delft Method [16]

***Step1*: Properties data**

Before the design of distillation column, some important data such as liquid and vapor density, surface tension and velocity at different location of the column need to be calculated.

1. Calculation of the density of liquid and vapor

a) The liquid density can be obtained from Aspen simulation directly

Table A.5.7.1: Liquid density of the top and bottom products

Top	0.854728	g/cc
Bottom	1.202778	g/cc

The liquid density does not change much at the different location of column.
The liquid density at feed stage can be estimated as 1 g/cc reasonably.

b) The vapor density is calculated from the mole composition c_i of each substance and the density ρ_i of each substance: $\rho = \sum_i \rho_i c_i$

ρ_i is calculated based on the ideal gas state equation: $\rho_i = \frac{PM_i}{RT}$

Table A.5.7.2: Temperature data of several stages in the column

P	15198.75 Pa	0.15 atm
T_{top}	326.87 K	53.72 °C
T_{stage9}	327.78 K	
$T_{stage10}$	328.52 K	
T_{bottom}	371.37 K	98.21 °C

Table A.5.7.3: Molecular weight of components

Substance	M_i	*Remarks*
Propenea	100	In the 'substance' column, some abbreviations are used to write the chemical name shortly. The full name of the abbreviations is given as the following (these abbreviations will be used in this chapter): (1) Propena means propenyl acetate (2) Precursor means (R)-3-chloro-1-phenylpropyl acetate (3) Reactant means R-, S- 3-chloro-1-phenyl-1-propanol (4) Isopro means Isopropanol
Precursor	212.5	
Reactant	170.5	
Acetone	58.08	
Toluene	92.1405	
Water	18	
Isopro	60.0959	

c_i (vapor mole composition) is from the Aspen simulation ; The density at different stages are calculated as shown in the following table:

Table A.5.7.4: Calculation of density of some stages in the column

Substance (i)	*Density for sub. Top* ρ_i	*Liq. mole composition Top* c_i	*Density Top (g/m³)* ρ	*Density for sub. Stage9* ρ_i	*Liq mole composition Stage9* c_i	*Density Stage9 (g/m³)* ρ
Propenea	559.2591	0.019777	11.06047	557.7155	0.016212	9.041813
Precursor	1188.426	1.23E-04	0.145713	1185.146	0.00564	6.684221
Reactant	953.5368	2.36E-29	2.25E-26	950.905	6.96E-11	6.62E-08
Acetone	324.8177	0.039435	12.80911	323.9212	0.027765	8.993688
Toluene	515.3041	0.927337	477.8606	513.8819	0.941191	483.6612
Water	100.6666	0.004444	0.447321	100.3888	0.003012	0.302375
Isopro	336.0918	0.008885	2.986145	335.1642	0.006179	2.071097
Total		1	505.3094		1	510.7544

Table A.5.7.4 (continued):

Substance (i)	*Density for sub. Stage10* ρ_i	*Liq. mole composition Stage10* c_i	*Density Stage10 (g/m³)* ρ	*Density for sub. Bottom* ρ_i	*Liq. mole composition Bottom* c_i	*Density Bottom (g/m³)* ρ
Propenea	556.4559	0.014557	8.100301	492.2583	9.20E-07	4.53E-04
Precursor	1182.469	0.008452	9.994001	1046.049	0.92536813	9.68E+02
Reactant	948.7573	2.93E-08	2.78E-05	839.3003	5.66E-07	4.75E-04
Acetone	323.1896	0.013205	4.267841	285.9036	5.23E-13	1.50E-10
Toluene	512.7212	0.961307	492.8824	453.5692	0.07463038	3.39E+01
Water	100.1621	9.01E-05	0.009022	88.60649	2.73E-29	2.41E-27
Isopro	334.4072	0.002389	0.798912	295.827	5.47E-16	1.62E-13
Total		1	516.0525		1	1.00E+03

2. Calculation of surface tension, σ (obtained from Aspen simulation)

Table A.5.7.5: Calculation of surface tension of some stages in the column

Substance (i)	σ_i *for sub. top*	*Mole composition top*	σ *Top (N/m)*	σ_i *for sub. Stage9*	*Mole composition Stage9*	σ *Stage9 (N/m)*
Propenea	0.021459	0.011061	0.000237	0.021358	0.008649	0.000185
Precursor	0.034197	0.000598	2.05E-05	0.034124	0.02607	0.00089
Reactant	0.046791	3.26E-26	1.53E-27	0.046685	9.23E-08	4.31E-09
Acetone	0.01953	0.004695	9.17E-05	0.019421	0.003323	6.45E-05
Toluene	0.024563	0.98289	0.024143	0.024459	0.96144	0.023516
Water	0.067163	1.30E-05	8.76E-07	0.066987	1.07E-05	7.14E-07
Isopro	0.018744	0.000742	1.39E-05	0.018671	0.000508	9.48E-06
Total		1	0.024507		1	0.024665

Table A.5.7.5 (continued):

Substance (i)	σ_i *for sub. Stage10*	*Mole Composition Stage10*	σ *Top (N/m)*	σ_i *for sub. bottom*	*Mole Composition bottom*	σ *bottom (N/m)*
Propenea	0.021275	0.00749	0.000159	0.016576	1.79E-08	2.97E-10
Precursor	0.034064	0.0376	0.001283	0.030596	0.994394	3.04E-02
Reactant	0.046599	3.71E-05	1.73E-06	0.041599	0.001255	5.22E-05
Acetone	0.019331	0.00156	3.02E-05	0.014233	1.90E-15	2.71E-17
Toluene	0.024374	0.953	0.023229	0.01954	0.00435	8.50E-05
Water	0.066843	3.37E-07	2.25E-08	0.058558	3.40E-33	1.99E-34
Isopro	0.018611	0.000191	3.56E-06	0.015023	4.79E-19	7.19E-21
Total		1.00	0.024707		1.00	0.0306

3. The mass flow rate (M_L) of liquid and mass flow rate (M_G) of vapor (obtained from Aspen simulation)
Here stage1 is total condenser, stage 9 is feed stage and the stage 22 is the reboiler. So inside the column, there are 20 stages:

Table A.5.7.6: Liquid (M_L) and gas (M_G) mass flow rate

stage	M_L(kg/s)	M_G(kg/s)
1	0.085923	0
2	0.094238	0.276862
3	0.094439	0.285178
4	0.094478	0.285378
5	0.094526	0.285417
6	0.094598	0.285465
7	0.094709	0.285538
8	0.094875	0.285648
9	0.095117	0.285814

Table A.5.7.6 (continued)

stage	M_L(kg/s)	M_G(kg/s)
10	0.273644	0.252019
11	0.274134	0.255943
12	0.274227	0.256433
13	0.274295	0.256526
14	0.274488	0.256594
15	0.275249	0.256787
16	0.278218	0.257549
17	0.287585	0.260518
18	0.305783	0.269884
19	0.327064	0.288082
20	0.344325	0.309363
21	0.352678	0.326624
22	0.017701	0.334977

Step 2: ***Dimension of column***

The operation condition is different at the different position in the column. Four positions are chosen to make the calculation for the column diameter, i.e.: top, stage9, stage10 (feed stages), and bottom. The final diameter can be decided from these four calculation results.

In the following procedure, the stage 9 is taken to make the calculation example

1. Flow parameter F_{LG} is a basic factor for design:

$$F_{LG} = \frac{M_L}{M_G}\sqrt{\frac{\rho_G}{\rho_L}} = \frac{u_{Ls}}{u_{Gs}}\sqrt{\frac{\rho_G}{\rho_L}} \qquad F_{LG,stage9} = \frac{0.09512}{0.2858}\sqrt{\frac{0.510}{1000}} = 0.00752$$

the graph

Figure A.5.7.1: Plot of F_{LG} vs C_G (taken from the Delft Method) [16]

From the graph, according to F_{LG}, the capacity factor c_G can be determined

So, when $F_{LG} = 0.00752$, c_G =0.08.

2 The maximum allowable gas velocity

$$u_{G,\max} = c_G\sqrt{\frac{\rho_L - \rho_G}{\rho_G}}\left(\frac{\sigma}{0.02}\right)^{0.2} \qquad u_{G,\max,stage9} = 3.694 m/s$$

3 Normally $u_{G,oper} = 0.8 u_{G,\max}$

$$u_{G,oper,stage9} = 0.8 u_{G,\max,stage9} = 2.955 m/s$$

4 Tentative column diameter (from continuity capacity):

$$d_c = \sqrt{\frac{4}{\pi}\frac{M_G}{\rho_G u_{G,oper}}} \qquad d_{c,stage9} = 0.49 m$$

The calculation results of other position is showed in the following table A5.7.7

Table A.5.7.7: Result of calculation of column diameter

d_{top}	0.50 m
d_{stage9}	0.49 m
$d_{stage10}$	0.47 m
d_{bottom}	0.50 m

The worst case is chosen for safety reason, therefore the diameter is 0.5 m.

5 Calculation of the area

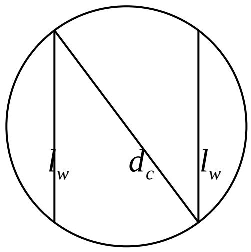
$$A_c = \pi \frac{d_c^2}{4} \qquad A_c = 0.196 m^2$$

6 According to the standard tray dimensions, in the vacuum condition

$$l_w = 0.55 d_c \qquad l_w = 0.275 m$$

7 Calculation of non-active area:

$$A_d \approx \frac{A_c - l_w^2}{4} \qquad A_d \approx 0.03 m^2$$



8 Calculation of active area

$$A_{ac} = A_c - 2A_d \qquad A_{ac} = 0.136 m^2$$

9 The holes area is 10% of the total area of tray

$$A_h = 0.1 A_{ac} \qquad A_h = 0.0136 m^2$$

11 The total height of trays in the column

$$h_{trays} = T_s (N_r - 1) \qquad h_{trays} = 0.45(20-1) = 8.55 m$$

12 According to the standard, the following is chosen:

$$h_{top} = 1.5 m \; ; \; h_{bottom} = 2.5 m \; ; h_{skirt} = 2m$$

13 The total height of column is summary of h_{trays} , h_{bottom} *and* h_{skirt}

$$h_c(m) = h_{tt} + h_{skirt} = h_{trays} + h_{bottom} + h_{skirt} \qquad h_c(m) = 14.55 m$$

Step 3 **Pressure drop check**

1. The superficial gas velocity

$$u_{Gs} = \frac{M_G}{\rho_G A_c} \qquad u_{Gs} = 3.225 m/s$$

2. The superficial liquid velocity

$$u_{Ls} = \frac{M_L}{\rho_L A_c} \qquad u_{Ls} = 0.0018 m/s$$

3. The gas velocity going through the holes in the tray

$$u_{Gh} = \frac{M_G}{\rho_G A_h} \qquad u_{Gh} = 46.56 m/s$$

4 The gas load is best expressed by so called F-factor:

$$F_G = u_{Gs}\sqrt{\rho_G} \qquad F_G = 2.317 Pa^{0.5}$$

5 Maximum gas load is derived from a balance of friction force and weight force minus buoyancy, taking into account drop stability via a critical Weber number

$$F_{G,\max} = 2.5(\phi^2 \sigma g(\rho_L - \rho_G))^{0.25} \qquad F_{G,\max} = 3.289 Pa^{0.5}$$

6 Liquid holdup:

$$\varepsilon_L = \frac{h_L}{h_f} = 1 - \left(\frac{F_G}{F_{G,\max}}\right)^{0.28} \qquad \varepsilon_L = 0.093$$

7 The weir height h_w is chosen as 0.03m according to the standard;

8 The froth height is given from the following formula:

$$h_f = h_w + \frac{1.45}{g^{1/3}}\left(\frac{u_{Ls}A_c}{l_w \varepsilon_L}\right)^{2/3} + \frac{125}{g(\rho_L - \rho_G)}\left(\frac{F_G - 0.2\sqrt{\rho_G}}{1-\varepsilon_L}\right)^2 \qquad h_f = 0.14m$$

9 Orifice coefficient, here experience data ς_0 is chosen as 2.67 according to the thin plate and relative free area ϕ is 0.1:

$$\varsigma = \varsigma_0 + \phi^2 - 2\phi\sqrt{\varsigma_0} \qquad \varsigma = 2.35$$

10 Dry tray pressure drop:

$$\Delta p_{dry} = \varsigma \frac{\rho_G u_{Gh}^2}{2} = \frac{\varsigma}{2} F_{Gh}^2 \qquad \Delta p_{dry} = 1316.23 Pa$$

11 Static liquid head:

$$\Delta p_L = h_L \rho_L g = \varepsilon_L h_f \rho_L g \qquad \Delta p_L = 130.25 Pa$$

12 The total pressure drop is summary of Δp_{dry} , Δp_L *and* Δp_r , Δp_r is pressure drop due to several so called residual factors, which often can be neglected.

$$\Delta p_t = \Delta p_{dry} + \Delta p_L + \Delta p_r \qquad \Delta p_t = 1446.48 Pa = 0.01 bara$$

So, the pressure drop along the column is very small. The above calculation result is acceptable.

A5.8 Design of heat exchangers E101-E104

A5.8.1 Heater for column feed E101

Table A5.8.1: Useful data for the design of heat exchange E101

E101	T_{in} (^oC)	T_{out} (^oC)	*Heat transfer* (kJ/s)	*Shell/Tube*
Hot stream (L.P steam)	110 (T_1)	110 (T_2)	25.2	Shell
Cold stream	20 (t_1)	88 (t_2)		Tube
Remarks: - refer to table A4.9, appendix A4.3.2 for the data used in this table				

Heat Load (from one of above Q's;)

Q = 25.2 kJ/s (table A5.8.1)

Logarithmic Mean Temperature Difference (ΔT_{lm})

$$\Delta T_{lm} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln \frac{(T_1 - t_2)}{(T_2 - t_1)}} = 48.27\ ^oC$$

where ΔT_{lm}: log mean temperature difference.
T_1: inlet shell-side fluid temperature.
T_2: outlet shell-side fluid temperature.
t_1: inlet tube-side temperature.
t_2: outlet tube-side temperature.

Heat Exchange area (A) For "single pass"-tube/"single pass"-shell combination.

General equation for heat transfer across a surface is:

$$Q = UA\Delta T_m$$

where: Q: heat transferred per unit time = 25.2 kJ/s = 25.2 [kW]
U: the overall heat transfer coefficient = 0.250 [$kW/m^2\ ^oC$]
A: heat-transfer area [m^2]
ΔT_m: the main temperature difference, the temperature driving force:

$$\Delta T_m = F_t \Delta T_{lm}$$

F_t = the temperature correction factor.

For "single pass"-tube/"single pass"-shell combination: $F_t = 1$ [15], hence $\Delta T_m = 48.27$

→ $A = 2.1\ m^2$

A5.8.2 Column's condenser E102

Table A5.8.2: Useful data for the design of heat exchange E102

E102	T_{in} (°C)	T_{out} (°C)	*Heat transfer* (kJ/s)	*Shell/Tube*
Hot stream	53.7 (T_1)	34 (T_2)	121.02	Shell
Cold stream (cold water)	20 (t_1)	30 (t_2)		Tube
Remarks: - refer to table A4.7, appendix A4.3.2 for the data used in this table				

Heat Load (from one of above Q's;)

Q = 121.02 kJ/s (table A5.8.2)

Logarithmic Mean Temperature Difference (ΔT_{lm})

$$\Delta T_{lm} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln \frac{(T_1 - t_2)}{(T_2 - t_1)}} = 18.43\ ^oC$$

where ΔT_{lm}: log mean temperature difference.
T_1: inlet shell-side fluid temperature.
T_2: outlet shell-side fluid temperature.
t_1: inlet tube-side temperature.
t_2: outlet tube-side temperature.

Heat Exchange area (A) For "single pass"-tube/"single pass"-shell combination.

General equation for heat transfer across a surface is:

$$Q = UA\Delta T_m$$

where: Q: heat transferred per unit time = 121.02 kJ/s = 121.02 [kW]
U: the overall heat transfer coefficient = 0.250 [kW/m^2 °C]
A: heat-transfer area [m^2]
ΔT_m: the main temperature difference, the temperature driving force:

$$\Delta T_m = F_t \Delta T_{lm}$$

F_t = the temperature correction factor.

For "single pass"-tube/"single pass"-shell combination: $F_t = 1$ [15], hence $\Delta T_m = 18.43$

→ A = 26.27 m^2

A5.8.3 Column's reboiler E103

Table A5.8.3: Useful data for the design of heat exchange E103

E103	T_{in} (^oC)	T_{out} (^oC)	*Heat transfer* (kJ/s)	*Shell/Tube*
Hot stream(L.P steam)	110 (T_1)	110 (T_2)	102.2	Shell
Cold stream	98.2 (t_1)	100.02 (t_2)		Tube
Remarks: - refer to table A4.6, appendix A4.3.2 for the data used in this table				

Heat Load (from one of above Q's;)

Q = 102.2 kJ/s (table A5.8.3)

Logarithmic Mean Temperature Difference (ΔT_{lm})

$$\Delta T_{lm} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln \dfrac{(T_1 - t_2)}{(T_2 - t_1)}} = 10.87\ ^oC$$

where
- ΔT_{lm}: log mean temperature difference.
- T_1: inlet shell-side fluid temperature.
- T_2: outlet shell-side fluid temperature.
- t_1: inlet tube-side temperature.
- t_2: outlet tube-side temperature.

Heat Exchange area (A) For "single pass"-tube/"single pass"-shell combination.

General equation for heat transfer across a surface is:

$$Q = UA\Delta T_m$$

where:
- Q: heat transferred per unit time = 102.202 kJ/s = 102.202 [kW]
- U: the overall heat transfer coefficient = 0.250 [kW/m^2 ^oC]
- A: heat-transfer area [m^2]
- ΔT_m: the main temperature difference, the temperature driving force:

$$\Delta T_m = F_t \Delta T_{lm}$$

F_t = the temperature correction factor.

For "single pass"-tube/"single pass"-shell combination: F_t = 1 [15], hence ΔT_m = 10.87

→ A = 37.63 m^2

A5.8.4 Product cooler E104

Table A5.8.4: Useful data for the design of heat exchange E104

E104	T_{in} (°C)	T_{out} (°C)	*Heat transfer* (kJ/s)	*Shell/Tube*
Hot stream	98.2 (T_1)	25 (T_2)	1.55	Shell
Cold stream (cold water)	20 (t_1)	30 (t_2)		Tube
Remarks: - refer to table A4.10, appendix A4.3.2 for the data used in this table				

Heat Load (from one of above Q's;)

Q = 1.55 kJ/s (table A5.8.4)

Logarithmic Mean Temperature Difference (ΔT_{lm})

$$\Delta T_{lm} = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln \frac{(T_1 - t_2)}{(T_2 - t_1)}} = 24.19\ ^{o}C$$

where
- ΔT_{lm}: log mean temperature difference.
- T_1: inlet shell-side fluid temperature.
- T_2: outlet shell-side fluid temperature.
- t_1: inlet tube-side temperature.
- t_2: outlet tube-side temperature.

Heat Exchange area (A) For "single pass"-tube/"single pass"-shell combination.

General equation for heat transfer across a surface is:

$$Q = UA\Delta T_m$$

where:
- Q: heat transferred per unit time = 1.55 kJ/s = 1.55 [kW]
- U: the overall heat transfer coefficient = 0.250 [kW/m^2 ^{o}C]
- A: heat-transfer area [m^2]
- ΔT_m: the main temperature difference, the temperature driving force:

$$\Delta T_m = F_t \Delta T_{lm}$$

F_t = the temperature correction factor.

For "single pass"-tube/"single pass"-shell combination: $F_t = 1$ [15], hence $\Delta T_m = 24.19$

→ A = 0.26 m^2

A5.9.1 Design of toluene transfer pump P101

Pump P101: Toluene transfer pump (refer to Process Flow Scheme, part 5.2, chapter5)

Toluene density at 25^0C = 866 kg/m^3 (refer to part 3.2.4, chapter 3 for pure component properties)
Viscosity: 0.9 mNs/m^2 (0.9 cp)

Estimation of pipe diameter required:

Typical velocity for liquid 2 m/s ([15], p.191)

Mass flow = $\frac{520.12}{0.167}\frac{kg}{h} = 3120.72\ \frac{kg}{h} = 0.867\frac{kg}{s}$ (refer to stream <3>, table 5.2, chapter 5)

Volumetric flow = $\frac{0.867kg/s}{866kg/m^3} = 0.001m^3/s$

Area of pipe= $\frac{volumetric\ flow}{velocity} = \frac{0.001m^3/s}{2m/s} = 0.0005m^2$

$Diameter\ of\ pipe = \sqrt{\left(0.0005\times\frac{4}{\pi}\right)} = 0.0252m$. Take diameter as 26mm.

Cross-sectional area= $\frac{\pi 26^2}{4} = 5.31\times10^{-4}m^2$

Pressure –drop calculation:

$fluid\ velocity = \frac{0.001}{0.000531} = 1.89m/s$

Friction loss (use fanning pressure drop equation):

$\Delta P = 4.13\times10^{10}G^{1.84}\mu^{0.16}\rho^{-1}d^{-4.84}$

where $\Delta P =$ pressure drop, kN/m^2 (kPa),
$G =$ flow rate, kg/s,
$\rho =$ density, kg/m^3,
$\mu =$ viscosity, mNm^{-2}s,
$d =$ pipe diameter, mm.

$\Delta P = 4.13\times10^{10}(0.867)^{1.84}(0.9\times10^{-3})^{0.16}(866)^{-1}(26)^{-4.84} = 1.6923kPa/m$

Take the higher value, and design for a maximum flow rate of 20 per cent above the normal (average) flow:

Friction loss at maximum flow = 1.6923×1.2^2 = <u>2.4365 kPa/m</u>

The loss through the bends and block values can be included in line pressure-loss calculation as an "equivalent length of pipe" ([21], chapter3)

All the bends will be taken as 90^0 elbows of standard radius, equivalent length =30d, and the valves as plug valves, fully open, equivalent length = 18d. Line to pump suction:

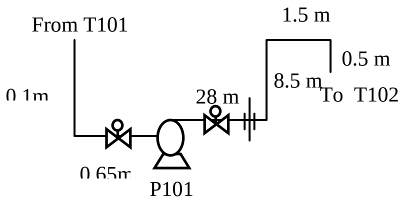


Figure A.5.9.1: Assumed length of pipes connected to pumps P101

Length = 0.75 = 0.75m
Bend, $1 \times 30 \times 26 \times 10^{-3}$ = 0.78m
Valve, $1 \times 18 \times 26 \times 10^{-3}$ = 0.47m
Total line length is 2m

Entry loss = $\frac{\rho u^2}{2}$ ([21], chapter3) at maximum design velocity = 2.1 kPa
(where maximum velocity =1.2 flow velocity)

Control valve pressure drop, allows normal		140kPa
	($\times 1.2^2$) maximum	200 kPa
Heat exchanger, allows normal		70 kPa
	($\times 1.2^2$) maximum	200 kPa
Orifice, allows normal		15 kPa
	($\times 1.2^2$) maximum	22 kPa

Line from pump discharge:

Length:	28 + 1.5 + 8.5 + 0.5 =	38.50m
Bend:	$3 \times 30 \times 26 \times 10^{-3}$ =	2.34 m
Valve:	$1 \times 18 \times 26 \times 10^{-3}$ =	0.47m
Total:		41.31m

See table A5.9.1 for line calculation sheet for pump P101 on next page.

Table A5.9.1: Pump P101 and line calculation sheet

PUMP P101 AND LINE CALCULATION SHEET									
Job no.	Sheet no.	By:				Checked:			
Fluid		Toluene			*Discharge calculation*				
Temperature©		25			Line size mm				
Density kg/m3		866				Flow	Norm.	Max.	Units
Viscosity mNs/m2		0.9				Velocity	1.89	2.2	m/s
Normal Flow kg/s		0.867				Friction loss	1.692	2.437	kPa/m
Design Max. Flow kg/s		1.0404				Line length	41.31		m
20% above the normal flow						Line loss	69.91	100.7	kPa
Suction Calculation						Orifice	15	22	kPa
Line size mm						Control Valve	140	200	kPa
	Flow	Norm.	Max.	Units		Equipment			
	Velocity	1.89	2.2	m/s		(a) Heat ex.			kPa
	Friction loss	1.692	2.4365	kPa/m		(b)			kPa
	Line length	2		m		(c)			kPa
	Line loss	3.384	4.873	kPa		**(6)** Dynamic Loss	224.9	322.7	kPa
	Entrance	1.54672	2.0957	kPa					
	Strainer			kPa		Static head	8		m
	(1) Sub-total	4.93072	6.9687	kPa			67.89		kPa
						Equip Press (Max)	100	100	kPa
	Static head	0.1		m		Contingency	None	None	kPa
		0.84868		kPa		**(7)** Subtotal	167.9	167.9	kPa
	Equip. Press	100	100	kPa	(7)+(6)	Discharge Press (p_d)	392.8	490.6	kPa
	(2) Sub-total	100.849	100.85	kPa		Suction Press	95.92	93.88	kPa
(2)-(1)	**(3)** Suction Press	95.918	93.88	kPa		**(8)** Diff. Press	296.9	396.7	kPa
	(4) VAP.PRESS			kPa			39.98	53.41	m
(3)-(4)	**(5)** NPSH			kPa		Control Valve			
				m	Valve/(6)	%Dyn. Loss			

The type of the pump is chosen based on the capacity range and typical head of water ([15] table 10.17, p434). In this case, the capacity is 3.6 m^3/h and the head is 53 m of water. Therefore, centrifugal pump is chosen (capacity range is 0.25-1000m^3/h, typical head is 10-50m of water (single stage) 300m of water (multistage))

Theoretical Pressure = $\Phi_v \cdot (p_d - p_s) \cdot 10^2$ = 0.4 kW.

The efficiency is found to be 27% (from figure 10.62, p435, [15])

Therefore the power at shaft is 1.5 kW

A5.9.2 Design of liquid transport pump P102

The detail calculation is the same as the calculation in appendix A5.9.1 for pump P101 (toluene transfer pump design)

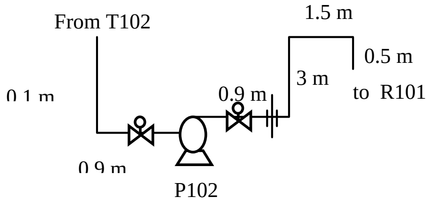


Figure A.5.9.2: Assumed length of pipes connected to pumps P102

Table A5.9.2: Pump P102 and line calculation sheet

PUMP P102 AND LINE CALCULATION SHEET									
Job no.	Sheet no.	By:			Checked:				
Fluid		Toluene /Catalyst			*Discharge calculation*				
Temperature©		20			Line size mm				
Density kg/m3		873.6				Flow	Norm.	Max.	Units
Viscosity mNs/m2		0.9				Velocity	1.97	2.2	m/s
Normal Flow kg/s		1.7527				Friction loss	1.268	1.826	kPa/m
Design Max. Flow kg/s		2.10324				Line length	8.74		m
20% above the normal flow						Line loss	11.09	15.97	kPa
Suction Calculation						Orifice	15	22	kPa
Line size mm						Control Valve	140	200	kPa
	Flow	Norm.	Max.	Units		Equipment			
	Velocity	1.97	2.2	m/s		(a) Heat ex.			kPa
	Friction loss	1.268	1.8259	kPa/m		(b)			kPa
	Line length	2.75		m		(c)			kPa
	Line loss	3.487	5.0213	kPa		**(6)** Dynamic Loss	166.1	238	kPa
	Entrance	1.69518	2.1141	kPa					
	Strainer			kPa		Static head	2.5		m
	(1) Sub-total	5.18218	7.1354	kPa			21.4		kPa
						Equip Press (Max)	100	100	kPa
	Static head	0.1		m		Contingency	None	None	kPa
		0.85613		kPa		**(7)** Subtotal	121.4	121.4	kPa
	Equip. Press	100	100	kPa	(7)+(6)	Discharge Press	287.5	359.4	kPa
	(2) Sub-total	100.856	100.86	kPa		Suction Press	95.67	93.72	kPa
(2)-(1)	**(3)** Suction Press	95.674	93.721	kPa		**(8)**Diff. Press	191.8	265.6	kPa
	(**4**) VAP.PRESS			kPa			25.83	35.77	m
(3)-(4)	**(5)** NPSH			kPa		Control Valve			
				m	Valve/(6)	%Dyn. Loss	84%		

Because the capacity is 7.2m^3/h Head is 36m of water. Centrifugal pump is chosen (capacity range is 0.25-1000m^3/h, typical head is 10-50m of water (single stage) 300m of water (multistage)) ([15], table 10.17, p434)

Theoretical Pressure = $\Phi_v \cdot (p_d - p_s) \cdot 10^2$= 0.52kW. ($\Phi_v$ is capacity of pump unit is m^3/s)

The efficiency is found to be 42% ([15] figure 10.62, p435)

Therefore the Power at shaft is 1.3kW

A5.9.3 Design of reaction mixture transport pump P103

The detail calculation is the same as the calculation in appendix A5.9.1 for pump P101 (toluene transfer pump design)

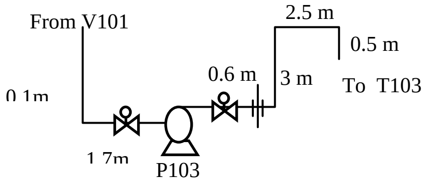


Figure A.5.9.3: Assumed length of pipes connected to pumps P103

Table A5.9.3: Pump P103 and line calculation sheet

PUMP P103 AND LINE CALCULATION SHEET									
Job no.	Sheet no.	By:				Checked:			
Fluid		Reaction mixture			*Discharge calculation*				
Temperature©		30			Line size mm				
Density kg/m^3		904.5				Flow	Norm.	Max.	Units
Viscosity mNs/m^2		0.9				Velocity	1.768	2	m/s
Normal Flow kg/s		0.5024				Friction loss	2.114	3.044	kPa/m
Design Max. Flow kg/s		0.60288				Line length	8.744		m
20% above the normal flow						Line loss	18.48	26.62	kPa
Suction Calculation			0.6m			Orifice	15	22	kPa
Line size mm						Control Valve	140	200	kPa
	Flow	Norm.	Max.	Units		Equipment			
	Velocity	1.768	2	m/s		(a) Heat ex.			kPa
	Friction loss	2.114	3.0442	kPa/m		(b)			kPa
	Line length	2.75		m		(c)			kPa
	Line loss	5.8135	8.3714	kPa		**(6)** Dynamic Loss	173.5	248.6	kPa
	Entrance	1.41365	1.809	kPa					
	Strainer			kPa		Static head	2.5		m
	(1) Sub-total	7.22715	10.18	kPa			22.16		kPa
						Equip Press (Max)	100	100	kPa
	Static head	0.1		m		Contingency	None	None	kPa
		0.88641		kPa		**(7)** Subtotal	122.2	122.2	kPa
	Equip. Press	100	100	kPa	(7)+(6)	Discharge Press	295.6	370.8	kPa
	(2) Sub-total	100.886	100.89	kPa		Suction Press	93.66	90.71	kPa
(2)-(1)	**(3)** Suction Press	93.6593	90.706	kPa		**(8)**Diff. Press	202	280.1	kPa
	(**4)** VAP.PRESS			kPa			27.2	37.71	m
(3)-(4)	**(5)** NPSH			kPa		Control Valve			
				m	Valve/(6)	%Dyn. Loss	81%		

Because the capacity is 1.99m^3/h Head is 37.71m of water. Centrifugal pump is chosen (capacity range is 0.25-1000m^3/h, typical head is 10-50m of water (single stage) 300m of water (multistage)) ([15], table 10.17, p434)

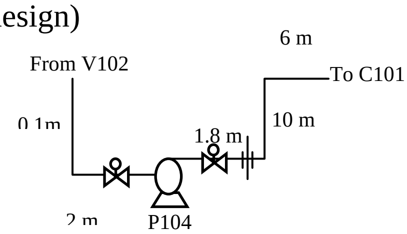
Theoretical Pressure = $\Phi_v \cdot (p_d - p_s) \cdot 10^2$= 0.15kW. ($\Phi_v$ is capacity of pump unit is m^3/s)

The efficiency is found to be 23% ([15] figure 10.62, p435).

Therefore the Power at shaft is 0.7kW.

A5.9.4 Design of column's feed transport pump P104

The detail calculation is the same as the calculation in appendix A5.9.1 for pump P101 (toluene transfer pump design)



<u>Figure A.5.9.4</u>: Assumed length of pipes connected to pumps P104

<u>Table A5.9.4</u>: Pump P104 and line calculation sheet

PUMP P104 AND LINE CALCULATION SHEET									
Job no.	Sheet no.	By:				Checked:			
Fluid		Reaction mixture			*Discharge calculation*				
Temperature©		20			Line size mm				
Density kg/m^3		897				Flow	Norm.	Max.	Units
Viscosity mNs/m^2		0.9				Velocity	1.752	2	m/s
Normal Flow kg/s		0.2086				Friction loss	3.404	4.902	kPa/m
Design Max.Flow kg/s		0.25032				Line length	19.31		m
20% above the normal flow						Line loss	65.72	94.64	kPa
Suction Calculation						Orifice	15	22	kPa
Line size mm						Control Valve	140	200	kPa
	Flow	Norm.	Max.	Units		Equipment			
	Velocity	1.752	2	m/s		(a) Heat ex.	70	100	kPa
	Friction loss	3.404	4.9018	kPa/m		(b)			kPa
	Line length	3.03		m		(c)			kPa
	Line loss	10.3141	14.852	kPa		**(6)** Dynamic Loss	290.7	416.6	kPa
	Entrance	1.37667	1.794	kPa					
	Strainer			kPa		Static Head	10		m
	(1) Sub-total	11.6908	16.646	kPa			87.91		kPa
						Equip Press (Max)	15	15	kPa
	Static head	0.1		m		Contingency	None	None	kPa
		0.87906		kPa		**(7)** Subtotal	102.9	102.9	kPa
	Equip. Press	100	100	kPa	(7)+(6)	Discharge Press	393.6	519.5	kPa
	(2) Sub-total	100.879	100.88	kPa		Suction Press	89.19	84.23	kPa
(2)-(1)	**(3)** Suction Press	89.1883	84.233	kPa		**(8)**Diff. Press	304.4	435.3	kPa
	(4) VAP.PRESS			kPa			40.99	58.62	m
(3)-(4)	**(5)** NPSH			kPa		Control Valve			
				m	Valve/(6)	%Dyn.Loss			

Because the capacity is 0.85m^3/h Head is 58.62m of water. Centrifugal pump is chosen (capacity range is 0.25-1000m^3/h, typical head is 10-50m of water (single stage) 300m of water (multistage)) ([15], table 10.17, p434)

Theoretical Pressure = $\Phi_v \cdot (p_d - p_s) \cdot 10^2$= 0.11kW. ($\Phi_v$ is capacity of pump unit is m^3/s)

The efficiency is found to be 17% ([15] figure 10.62, p435).

Therefore the Power at shaft is 0.7kW.

A5.9.5 Design of vacuum pump P105

The detail calculation is the same as the calculation in appendix A5.9.1 for pump P101 (toluene transfer pump design)

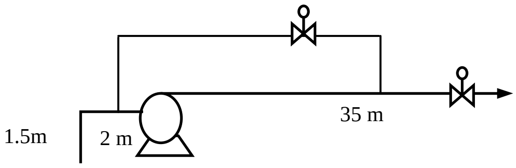


Figure A.5.9.5: Assumed length of pipes connected to pumps P105

Table A5.9.5: Pump P105 and line calculation sheet

PUMP P105 AND LINE CALCULATION SHEET									
Job no.	Sheet no.	By:			Checked:				
Fluid		Air			*Discharge calculation*				
Temperature©		100			Line size mm				
Density kg/m^3		1.2				Flow	Norm.	Max.	Units
Viscosity Ns/m^2		0.00002				Velocity	10	15	m/s
Normal Flow kg/s		0.01				Friction loss	0.07	0.10	kPa/m
Design Max. Flow kg/s		0.02				Line length	44	44	m
						Line loss	3.08	4.4	kPa
Suction Calculation						Orifice	15	22	kPa
Line size mm						Control Valve	140	200	kPa
	Flow	Norm.	Max.	Units		Equipment			
	Velocity	10	15	m/s		(a) Heat ex.			kPa
	Friction loss	0.07	0.07	kPa/m		(b)			kPa
	Line length	5	5	m		(c)			kPa
	Line loss	0.35	0.50	kPa		**(6)** Dynamic Loss	158.1	226.4	
	Entrance	0.06	0.14	kPa					
	Strainer			kPa		Static head	2	2	m
	(1) Sub-total	0.4	0.6	kPa			0.024	0.02	kPa
						Equip Press (Max)	100	100	kPa
	Static head	2	2	m		Contingency	None	None	kPa
		0.0	0.0	kPa		**(7)** Subtotal	100	100.0	kPa
	Equip. Press	15	15	kPa	(7)+(6)	Discharge Press	258.1	326.5	kPa
	(2) Sub-total	15.0	15.0	kPa		Suction Press	14.61	14.4	kPa
(2)-(1)	**(3)** Suction Press	14.6	14.4	kPa		**(8)** Diff. Press	243.5	312.1	kPa
	(**4)** VAP.PRESS	0.1	0.1	kPa					m
(3)-(4)	**(5)** NPSH	14.5	14.3	kPa		Control Valve			
		1234.1	1214.7	m	Valve/(6)	%Dynamic loss	89%		

To create 0.15bar, Rotary pump is used, according to Perry's chemical engineering handbook ([13] refer to figure 10-105: Vacuum levels attainable with various types of equipment. P10-59)

The capacity is 0.008m^3/s and the difference pressure is 312.1kPa.

Theoretical pressure = $\Phi_v \cdot (p_d - p_s) \cdot 10^2$= 2.5kW. ($\Phi_v$ is capacity of pump unit is m^3/s)

The efficiency of reciprocating pumps is usually around 90% ([15] p435) Assume that the efficiency of rotary pump is 90%. Therefore the Power at shaft is 2.8kW

A5.9.6 Design of toluene reflux pump P106

The detail calculation is the same as the calculation in appendix A5.9.1 for pump P101 (toluene transfer pump design)

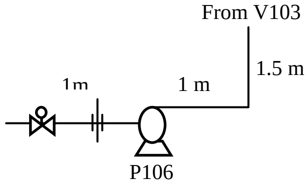


Figure A.5.9.6: Assumed length of pipes connected to pumps P106

Table A5.9.6: Pump P106 and line calculation sheet

PUMP P106 AND LINE CALCULATION SHEET									
Job no.	Sheet no.	By			Checked				
Fluid		Toluene			*Discharge calculation*				
Temperature©		34			Line size mm				
Density kg/m^3		854.7				Flow	Norm.	Max.	Units
Viscosity Ns/m^2		0.0001				Velocity	1	1.5	m/s
Normal Flow kg/s		0.0855				Friction loss	1.03	1.48	kPa/m
Design Max. Flow kg/s		0.1				Line length	1.5	1.5	m
						Line loss	1.545	2.22	kPa
Suction Calculation						Orifice	15	22	kPa
Line size mm						Control Valve	140	200	kPa
	Flow	Norm.	Max.	Units		Equipment			
	Velocity	1	1.5	m/s		(a) Heat ex.			kPa
	Friction loss	1.03	1.48	kPa/m		(b)			kPa
	Line length	3	3	m		(c)			kPa
	Line loss	3.09	4.4496	kPa		**(6)** Dynamic Loss	156.5	224.2	
	Entrance	0.4	1.0	kPa					
	Strainer			kPa		Static head	-0.4	-0.4	m
	(1) Sub-total	3.5	5.4	kPa			-3.35	-3.35	kPa
						Equip Press(Max)	15	15	kPa
	Static head	1.5	2.4	m		Contingency	None	None	kPa
		12.6	20.1	kPa		**(7)** Subtotal	11.65	11.65	kPa
	Equip. Press	15.0	15.0	kPa	(7)+(6)	Discharge Press	168.2	235.9	kPa
	(2) Sub-total	27.6	35.1	kPa		Suction Press	24.05	29.69	kPa
(2)-(1)	**(3)** Suction Press	24.0	29.7	kPa		**(8)**Diff. Press	144.1	206.2	kPa
	(4) VAP.PRESS	0.1	0.1	kPa			17.21	24.62	m
(3)-(4)	**(5)** NPSH	23.9	29.6	kPa		Control Valve			
		2.9	3.5	m	Valve/(6)	%Dynamic loss	89%		

Because the capacity is 0.4m^3/h Head is 24.62m of water. Centrifugal pump is chosen (capacity range is 0.25-1000m^3/h, typical head is 10-50m of water (single stage) 300m of water (multistage)) ([15] table 10.17, p434)

Theoretical Pressure = $\Phi_v \cdot (p_d - p_s) \cdot 10^2$= 0.021kW. ($\Phi_v$ is capacity of pump unit is m^3/s)

The efficiency is found to be 20% (from figure 10.62, p435, [15])

Therefore the Power at shaft is 0.11kW

A5.9.7 Design of technical grade toluene transport pump P107

The detail calculation is the same as the calculation in appendix A5.9.1 for pump P101 (toluene transfer pump design)

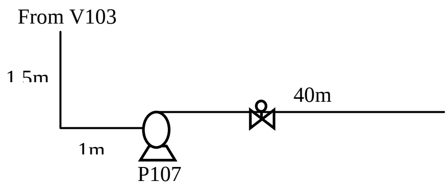


Figure A.5.9.7: Assumed length of pipes connected to pumps P107

Table A5.9.7: Pump P107 and line calculation sheet

PUMP P107 AND LINE CALCULATION SHEET									
Job no.	Sheet no.	By:			Checked:				
Fluid		Toluene			*Discharge calculation*				
Temperature©		34			Line size mm				
Density kg/m^3		854.7				Flow	Norm.	Max.	Units
Viscosity Ns/m^2		0.0001				Velocity	2	2.2	m/s
Normal Flow kg/s		0.19				Friction loss	3	4.32	kPa/m
Design Max. Flow kg/s		0.25				Line length	44	44	m
						Line loss	132	190.1	kPa
Suction Calculation						Orifice	15	22	kPa
Line size mm						Control Valve	140	200	kPa
	Flow	Norm.	Max.	Units		Equipment			
	Velocity	2	2.2	m/s		(a) Heat ex.			kPa
	Friction loss	3	4.32	kPa/m		(b)			kPa
	Line length	3	3	m		(c)			kPa
	Line loss	9	12.96	kPa		**(6)** Dynamic Loss	287	412.1	
	Entrance	1.7	2.1	kPa					
	Strainer			kPa		Static head	-13.5	-13.5	m
	(1) Sub-total	10.7	15.0	kPa			-113	-113	kPa
						Equip Press (Max)	100	100	kPa
	Static head	1.5	2.4	m		Contingency	None	None	kPa
		12.6	20.1	kPa		**(7)** Subtotal	-13.1	-13.1	kPa
	Equip. Press	15.0	15.0	kPa	(7)+(6)	Discharge Press	273.9	399	kPa
	(2) Sub-total	27.6	35.1	kPa		Suction Press	16.85	20.07	kPa
(2)-(1)	**(3)** Suction Press	16.9	20.1	kPa		**(8)**Diff. Press	257.1	378.9	kPa
	(4) VAP.PRESS	0.1	0.1	kPa			30.69	45.24	m
(3)-(4)	**(5)** NPSH	16.8	20.0	kPa		Control Valve			
		2.0	2.4	m	Valve/(6)	%Dyn. Loss	49%		

Because the capacity is 0.8m^3/h Head is 45.24m of water. Centrifugal pump is chosen (capacity range is 0.25-1000m^3/h, typical head is 10-50m of water (single stage) 300m of water (multistage)) ([15], table 10.17, p434)

Theoretical Pressure = $\Phi_v \cdot (p_d - p_s) \cdot 10^2$= 0.09kW. ($\Phi_v$ is capacity of pump unit is m^3/s)

The efficiency is found to be 20% ([15] figure 10.62, p435)

Therefore the Power at shaft is 0.45kW

A5.9.8 Design of product (precursor of Prozac) transport pump P108

The detail calculation is the same as the calculation in appendix A5.9.1 for pump P101 (toluene transfer pump design)

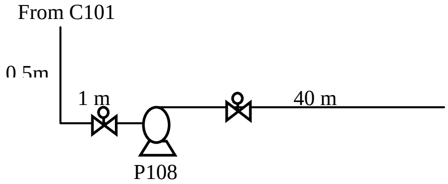


Figure A.5.9.8: Assumed length of pipes connected to pumps P108

Table A5.9.8: Pump P108 and line calculation sheet

PUMP AND LINE CALCULATION SHEET									
Job no.	Sheet no.	By:			Checked:				
Fluid		Product			*Discharge calculation*				
Temperature©		100			Line size mm				
Density kg/m3		1202.8				Flow	Norm.	Max.	Units
Viscosity Ns/m2		0.0003				Velocity	0.2	0.5	m/s
Normal Flow kg/s		0.02				Friction loss	0.54	0.78	kPa/m
Design Max.Flow kg/s		0.05				Line length	44	44	m
						Line loss	23.76	34.2	kPa
Suction Calculation						Orifice	15	22	kPa
Line size mm						Control Valve	140	200	kPa
	Flow	Norm.	Max.	Units		Equipment			
	Velocity	0.2	0.5	m/s		(a) Heat ex.	70	100	kPa
	Friction loss	0.54	0.78	kPa/m		(b)			kPa
	Line length	2.5	2.5	m		(c)			kPa
	Line loss	1.35	1.94	kPa		**(6)** Dynamic Loss	248.8	356.2	
	Entrance	0.02	0.15	kPa					
	Strainer			kPa		Static head	2	2	m
	(1) Sub-total	1.4	2.1	kPa			23.57	23.57	kPa
						Equip Press (Max)	100	100	kPa
	Static head	4	4	m		Contingency	None	None	kPa
		47.1	47.1	kPa		**(7)** Subtotal	123.6	123.6	kPa
	Equip. Press	15	15	kPa	(7)+(6)	Discharge Press	372.3	479.8	kPa
	(2) Sub-total	62.1	62.1	kPa		Suction Press	60.78	60.1	kPa
(2)-(1)	**(3)** Suction Press	60.8	60.1	kPa		**(8)** Diff. Press	311.6	419.7	kPa
	(4) VAP.PRESS	0.1	0.1	kPa			26.43	35.61	m
(3)-(4)	**(5)** NPSH	60.7	60.0	kPa		Control Valve			
		5.1	5.1	m	Valve/(6)	%Dyn. Loss	56%		

Because the capacity is $0.06m^3/h$ Head is 35.61m of water. Diaphragm pump is chosen (capacity range is $0.05\text{-}50m^3/h$, typical head is 5-60m of water) ([15], table 10.17, p434)

Theoretical Pressure = $\Phi_v \cdot (p_d - p_s) \cdot 10^2$= 0.0063kW. ($\Phi_v$ is capacity of pump unit is m^3/s)

Assume the efficiency of diaphragm is 50%. Therefore the Power at shaft is 0.013kW

APPENDIX A6 ECONOMY

A6.1 Prices of pumps

The prices for some centrifuge pumps are given in Dutch Association of Cost Engineers, *Prijzenboekje* (21st edition, Dec 2000, p35). However, the sizes of these pumps are not the same as the pumps required in the process. Based on the data given in the book, the correlations between power of the pumps and the prices, and also between the capacity and prices were studied.

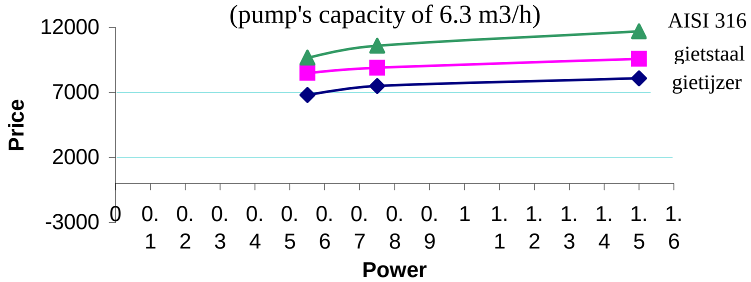
A6.1.1 The correlation between power and price

The pumps, which have the same capacity of 6.3m^3/h were studied

Table A6.1.1: Correlation between power and price (for the pumps' capacity of 6.3 m^3/h)

Capacity (m^3/h)	*Max power* (kW)	*Price* (Dfl)		
		AISI 316	gietijzer	gietstaal
6.3	0.55	9,700	6,800	8,500
	0.75	10,600	7,500	8,900
	1.50	11,700	8,100	9,600

Figure A6.1.1: PUMPS - Correlation between power and price (pump's capacity of 6.3 m3/h)



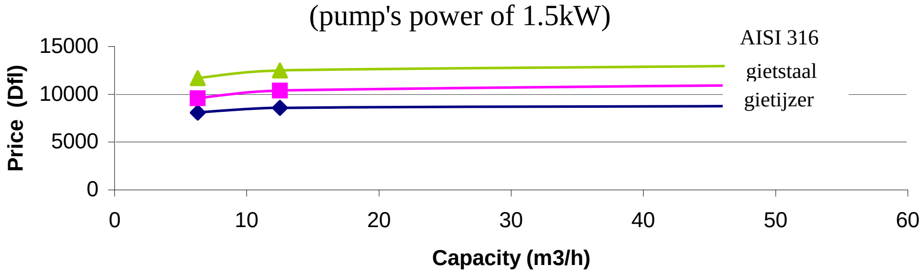
A6.1.2 The correlation between capacity and price

The pumps, which have the same power of 1.5kW were studied

Table A6.1.2: Correlation between capacity and price (for the pumps' power of 1.5kW)

Power (kW)	*Capacity* (m^3/h)	*Price* (Dfl)		
		AISI 316	gietstaal	gietijzer
1.5	6.3	11,700	9,600	8,100
	12.5	12,500	10,400	8,600
	50.0	13,000	11,000	8,800

Figure A6.1.2: PUMPS - Correlation between capacity and price (pump's power of 1.5kW)



It is found that the price will increase with the increase in capacity or power. There are not enough data so it is difficult to get high accuracy in the correlations between price, capacity and power.

A6.1.2 The capacity and price curve

The curve of price and capacity is produced from the price table in Dutch Association of Cost Engineers, *Prijzenboekje* (21st edition, Dec 2000, p35). For each type of pump's capacity the pumps, which have the highest power, are chosen for the determination of price. It means that if capacity is used to decide pumps' price, the pumps chosen will always have enough power compared to what needed for the certain duty in the plant.

Table A6.1.3: Correlation between capacity and price for the pumps with different power

Capacity (m^3/h)	*Price* (Dfl)		
	gietijzer	gietstaal	AISI 316
6.3	8,100	9,600	11,700
12.5	8,600	10,400	12,500
25	11,000	13,200	16,500
50	15,000	17,300	20,500
80	16,000	18,500	23,000
125	19,500	22,400	28,500
200	20,500	24,000	30,000
315	26,500	31,000	40,000

Figure A6.1.3: Capacity - Price curve for pumps with different power

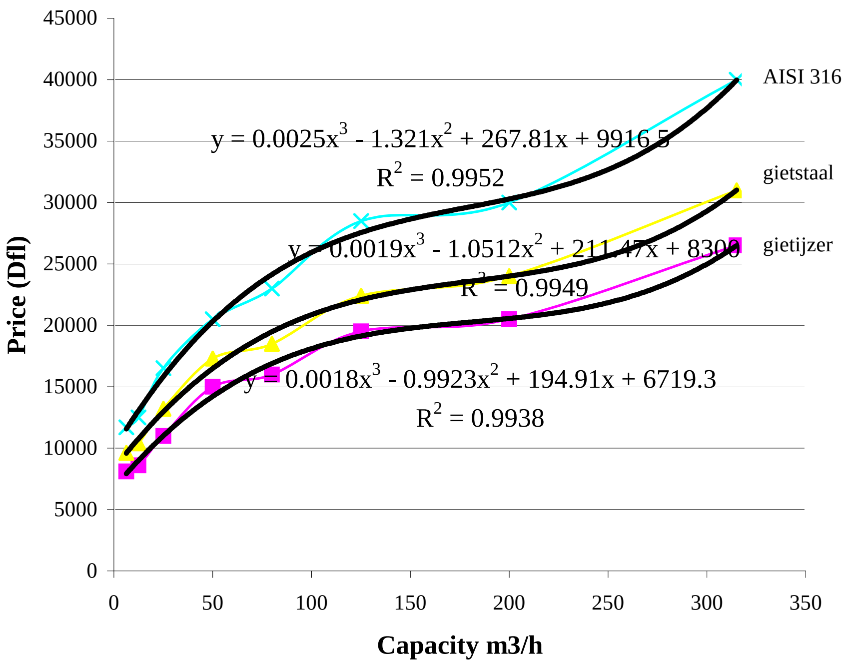


Figure A6.1.3 is used to determine the price of pumps

A6.2 Summary of equipment purchase costs

Table A6.2.1: Summary of purchase costs of dissolving and precipitation tanks, storage vessels and distillation column

Name	*Equipment*	*Type/ Figure/ Quantity.*	D (m) *Curve*	H (m) *Costs* (UK £)	M or C *Factor*	*Press.* (bar) *Factor*	*Costs equip.* (UK £)	*Costs Intern.* (UK £)	*Costs total* (UK £)	*Costs total* (Dfl)
T101	Vessel	Vertical	2	4.8	CS	1				
		fig.6-4	C3-	9,000	1	1	£9,000		£9,000	fl 27,000
T102	Vessel	Vertical	1	0.96	CS	1				
		fig.6-4	C2	2,000	1	1	£2,000		£2,000	fl 6,000
T103	Vessel	Vertical	1	1.07	CS	1				
		fig.6-4	C2	2,000	1	1	£2,000		£2,000	fl 6,000
V102	Vessel	Vertical	2.5	3.5	CS	1				
		fig.6-4	C3-+	8,400	1	1	£8,400		£8,400	fl 25,200
T104	Vessel	Vertical	3	11.2	CS	1				
		fig.6-4	C4-	26,000	1	1	£26,000		£26,000	fl 78,000
T105	Vessel	Vertical	1.5	2.4	CS	1				
		fig.6-4	C2-+	5,000	1	1	£5,000		£5,000	fl 15,000
C101	Vessel	Vertical	0.5	14.5	CS	0.15				
		fig.6-4	C1--	11,000	1	2.2	£24,200			
	Trays	Sieve	0.5		SS					
		fig. 6-6	C!							
		20		100	1.7		£3,400		£27,600	fl 82,800
Total	***Reactors** (T102, T103)*								**£4,000**	**fl 12,000**
	Storage vessels (T101, V102, T104, T105)								**£48,400**	**fl 145,200**
	***Column** (C101)*								**£27,600**	**fl 82,800**

Remarks:
- The figure used in the table are from J. M. Coulson & J. F. Richarson, 1979, *Chemical Engineering*, volume 6, p 223-224
- Pressure factor of column is estimated as same as the factor when pressure is 50-60 bar
- The rate of exchange (ROE) between Dfl and UK £ is 3.0

Table A6.2.2: Summary of purchase costs of the reactor and buffer tanks

Reactor& Vessels @ 1992

Name	*Equip.*	*Type*	*Capacity* (m^3) S	*Constant* C	*Index* n	*Comment*	*Equation*	*Cost* (UK £) Ce	*Cost total* (UK £)	*Cost total* (Dfl)
R101	Reactor	Jacketed	0.84	£8,000	0.4	CS	$Ce=CS^n$	£7,461	£7,461	fl 22,383
V101	Vessel	Vertical	0.4	£1,250	0.6	CS	Ce=CSn	£721	£721	fl 2,164
V103	Vessel	Vertical	1.44	£1,250	0.6	CS	$Ce=CS^n$	£1,567	£1,567	fl 4,702
Total	***Reactor** (R101)*								**£7,461**	**fl 22,383**
	Buffer tanks (V101, V103)								**£2,289**	**fl 6,866**

Remarks:
- The equation is from J. M. Coulson & J. F. Richarson, 1979, *Chemical Engineering*, volume 6, p225;
- The capacities of reactor and vessels are not fit the range for the equation, but assume the equation still can be used
- The rate of exchange (ROE) between Dfl and UK £ is 3.0

Table A6.2.3: Summary of purchase costs of heat exchangers and filters

Heat exchangers & Filters @1992										
Name	M of C Sh/Tubes	*Curve* (in fig.6-3	*Surface* (m^2)	*Cost* (UK £)	*Type*	*Factor*	*Press.* (bar)	*Factor*	*Cost* (UK £)	*Cost* (Dfl)
E101	CS/Brass	c2	2.1	£500	Float Hd.	1.0	1	1	£500	fl 1,500
E102	CS/Brass	c2	28.4	£8,000	Float Hd.	1.0	0.15	1.5	£12,000	fl 36,000
E103	CS/Brass	c2	37.63	£10,000	Float Hd.	1.0	0.15	1.5	£15,000	fl 45,500
E104	CS/Brass	c2	0.26	£54.76	Float Hd.	1.0	1	1	£54.76	fl 164
F101	-	-	80	$200	Micro-filter	1.0	1	1	$16,000	fl 48,000
F102	-	-	80	$200	Micro-filter	1.0	1	1	$16,000	fl 48,000
Total	***Heat exchanger**s (@1992)*								**£27,555**	**fl 82,664**
	Micro-filters' membrane (@ 2000)								**£22,080**	**fl 66,240**

Remarks:
- The figure 6.3 used in the table from J. M. Coulson & J. F. Richarson, 1979, *Chemical Engineering*, volume 6, p222
- The equation from J. M. Coulson & J. F. Richarson, 1979, *Chemical Engineering*, volume 6, p222
- Pressure factor of column is estimated as same as the factor when pressure is 50-60 bar
- The ROE between UK£ and US$ is 0.69 for www.gkw.nl,17/11/2001,15:00
- The ROE between Dfl and UK£ is 3.0
- The price of filter membrane comes from SUPERPRO program. It is the cost of membrane part for the micro-filter

Table A6.2.4: Summary of purchase costs of pumps

Pumps @ 2000							
Name	*Equipment*	*Type*	*Figure* (Appendix A6.1)	*Capacity* (m^3/h)	*Comment*	*Price* (Dfl/Pump)	*Total cost* Dfl
P101	Pump	Centrifugal	Figure A6.1.3	3.6	gietijzer	fl 7,408	fl 14,816
P102	Pump	Centrifugal	Figure A6.1.3	7.2	gietijzer	fl 8,072	fl 16,144
F101	Pump	Centrifugal	Figure A6.1.3	1.6	gietijzer	fl 7,029	fl 14,057
P103	Pump	Centrifugal	Figure A6.1.3	1.99	gietijzer	fl 7,103	fl 14,207
F102	Pump	Centrifugal	Figure A6.1.3	1.6	gietijzer	fl 7,029	fl 14,057
P104	Pump	Centrifugal	Figure A6.1.3	0.85	gietijzer	fl 6,884	fl 13,769
P105	Pump	Rotary	Figure A6.1.3	28.8	gietijzer	fl 11,553	fl 23,105
P106	Pump	Centrifugal	Figure A6.1.3	0.36	gietijzer	fl 6,789	fl 13,579
P107	Pump	Centrifugal	Figure A6.1.3	0.79	gietijzer	fl 6,873	fl 13,745
P108	Pump	Diaphragm	Figure A6.1.3	0.036	gietijzer	fl 6,726	fl 13,453
Total	***Pumps***						**fl 122,817**
	Micro-filters						**fl 28,114**

Remarks:
- The figure used to calculate the price of pumps is from appendix A6.1
- All the pumps have spares so factor 2 is used to calculate the total cost
- The pumps of F101 and F102 are part of micro-filter so the cost here is the pumps' cost for micro-filter.

A6.3 Capital investment cost calculation

From the purchased equipment costs (refer to appendix A6.2 for summary of equipment cost) the following terms is calculated: *Direct Capital*, *Indirect Capital Costs* and *Fixed Capital Costs* in UK@1992 by escalating given totals to UK@2001 (approximate interest is 8% per year). Lang's method is used for calculation.

Table A6.3.1: Capital investment cost calculation

Purchased Equipment Costs (PEC)	
Items @ 1992	**Cost (UK £)**
Reactors	11,461
Columns	27,600
Heat Exchangers	27,561
Storage vessels & Buffer tanks	50,689
Purchased Equipment Costs @ 1992	**117,310**
Purchased Equipment Costs @ 2001 (a) (Index correction, UK, @ 1992-2001, 8% per year: 1.999)	**234,503**
Items @ 2000	
Filters	31,452
Pumps	40,939
Purchased Equipment Costs @ 2000	**72,391**
Purchased Equipment Costs @ 2001 (b) (Index correction, UK, @ 2000-2001, 8% per year: 1.08)	**78,182**
Total purchased Equipment Costs @ 2001 (a) + (b) (The measurement cost included in long factor 'Instruments')	**312,685**
Total Direct Capital Cost @ 2001 (Lang factor, process type "Fluids": 3.4 with respect to PEC)	**1,063,129**
Total Indirect Capital Cost @ 1992 (Lang factor, process type "Fluids": 0.45 with respect to PPC)	**478,408**
Fixed Capital Costs @ 1992 (Total Direct Capital Cost + Total Indirect Capital Cost)	**1,541,537**
Total Direct Capital Cost @ 2001 (Dfl) (ROE=3.0)	**3,189,388**
Total Indirect Capital Cost @ 2001 (ROE=3.0)	**1,435,224**
Fixed Capital Costs @ 2001 (ROE=3.0)	**4,624,612**
Fixed Capital Costs @ 2001 (Euro) (ROE=2.2)	**2,102,096**
The Lang's factors from J. M. Coulson & J. F. Richarson, 1979, *Chemical Engineering*, volume 6 (chapter 6, table 6.1 of typical factors for estimation of project fixed capital cost)	

Remarks:
- Rate of exchange (ROE) between Dfl and UK £ is 3.0
- Rate of exchange (ROE) between Dfl and Euro is 2.2

A6.4 Discounted Cash Flow Rate of Return (DCFROR)

Table A6.4.1 Net present and future values for interest of 8%

END YEAR NO.	NET FUTURE VALUES (1) No Discount: CAPIT. COSTS ANN. (kDfl)	ACCUM. (kDfl)	CASH FLOW ANN. (kDfl)	ACCUM. (kDfl)	NFV (kDfl)	NET PRESENT VALUES Discounted, Accumulated: DISC. FACT. Interest 8.0%	CAPIT. COSTS ACCUM. (kDfl)	CASH FLOW ACCUM. (kDfl)	NPV (kDfl)
1	5,197	**5,197**			-5,197	1.000	**5,197**	5,197.0	-5,197
2			4,694	4,694	-503	0.926		4,346.3	-850.7
3			4,694	9,388	4,191	0.857		8,370.6	3173.6
4			4,694	14,082	8,885	0.794		12,096.9	6899.9
5			4,694	18,776	13,579	0.735		15,547.1	10350.1
6			4,694	23,470	18,273	0.681		18,741.8	13544.8
7			4,694	28,164	22,967	0.630		21,699.8	16502.8
8			4,694	32,858	27,661	0.583		24,438.7	19241.7
9			4,694	37,552	32,355	0.540		26,974.7	21777.7
10			4,694	42,246	37,049	0.500		29,322.9	24125.9
11			4,694	46,940	41,743	0.463		31,497.1	26300.1
ACCUM.		**5,197**		**46,940**	**41,743**	7.710	**5,197**	**31,497**	**26,300**
RATIO:				[Cash Flow / Capital] @ Disc.				**6.1**	
NET PRESENT VALUE:				[Cash Flow - Capital] @ Disc.				**26,300**	

N.B. :
1. Cash Flows "Before Tax".
2. Earning Power = Interest, for which [Cash Flow - Capital]@Disc. = 0
Disc. Factor = $1/(1 + r)^n$ with r = interest fraction

Table A6.4.2 Net present and future values for interest of 90.2%

END YEAR NO.	NET FUTURE VALUES (1) No Discount					NET PRESENT VALUES Discounted, Accumulated			
	CAPIT. COSTS		CASH FLOW			DISC. FACT. @	CAPIT. COSTS ACCUM.	CASH FLOW ACCUM.	
	ANN.	ACCUM.	ANN.	ACCUM.	**NFV**				**NPV**
	kDfl	kDfl	kDfl	kDfl	kDfl	**90.2%**	kDfl	kDfl	kDfl
1	5,197	**5,197**			-5,197	1.000	**5,197**	5,197	-5,197
2			4,694	4,694	-503	0.526		2,468	-2,729
3			4,694	9,388	4,191	0.276		3,765	-1,432
4			4,694	14,082	8,885	0.145		4,448	-749
5			4,694	18,776	13,579	0.076		4,806	-391
6			4,694	23,470	18,273	0.040		4,995	-202
7			4,694	28,164	22,967	0.021		5,094	-103
8			4,694	32,858	27,661	0.011		5,146	-51
9			4,694	37,552	32,355	0.006		5,174	-23
10			4,694	42,246	37,049	0.003		5,188	-9
11			4,694	46,940	41,743	0.002		5,197	0
ACCUM.		**5,197**		**46,940**	**41,743**	2.107	**5,197**	**5,197**	**0**
RATIO		**:**	[Cash Flow / Capital] @ Disc.					**1.0**	
NET PRESENT VALUE		**:**	[Cash Flow - Capital] @ Disc.					**0**	

N.B. : 1. Cash-Flows "Before Tax".
2. Earning Power = Interest, for which [Cash Flow - Capital]@Disc. = 0
Disc. Factor = $1/(1 + r)^n$ with r = interest fraction

When interest is 90.2%, the [Cash Flow – Capital] = 0
DCFROR = 90.2%

A6.5 DCFROR when there is 20% in reduction of original amount catalyst

Table A6.5.1 Net present and future values for interest of 8% when there is 20% in reduction of original amount of catalyst

END YEAR NO.	NET FUTURE VALUES (1) No Discount					NET PRESENT VALUES Discounted, Accumulated			
	CAPIT. COSTS		CASH FLOW			DISC. FACT. Interest	CAPIT. COSTS ACCUM.	CASH FLOW ACCUM.	**NPV**
	ANN.	ACCUM.	ANN.	ACCUM.	**NFV**				
	KDfl	kDfl	kDfl	kDfl	kDfl	**8.0%**	kDfl	kDfl	kDfl
1	5,197	**5,197**			-5,197	1.000	**5,197**	5,197	-5,197
2			11,870	11,870	6,674	0.926		10,991.0	5794.4
3			11,870	23,741	18,544	0.857		21,167.9	15971.2
4			11,870	35,611	30,414	0.794		30,590.9	25394.3
5			11,870	47,481	42,285	0.735		39,315.9	34119.3
6			11,870	59,351	54,155	0.681		47,394.6	42198.0
7			11,870	71,222	66,025	0.630		54,874.9	49678.3
8			11,870	83,092	77,895	0.583		61,801.1	56604.5
9			11,870	94,962	89,766	0.540		68,214.3	63017.7
10			11,870	106,833	101,636	0.500		74,152.4	68955.8
11			11,870	118,703	113,506	0.463		79,650.6	74454.0
ACCUM.		**5,197**		**118,703**	**113,506**	7.710	**5,197**	**79,651**	**74,454**

RATIO : [Cash Flow / Capital] @ Disc. **15.3**

NET PRESENT VALUE : [Cash Flow - Capital] @ Disc. **74,454**

N.B. :
1. Cash-Flows "Before Tax".
2. Earning Power = Interest, for which [Cash Flow – Capital]@Disc. = 0
   Disc. Factor = $1/(1 + r)^n$ with r = interest fraction
3. Rest Value = 6.0% of Capital Investment

Table A6.5.2 Net present and future values for interest of 228.4% when there is 20% in reduction of original amount of catalyst

	NET FUTURE VALUES (1) No Discount					**NET PRESENT VALUES** Discounted, Accumulated			
END YEAR NO.	CAPIT. COSTS ANN. kDfl	CAPIT. COSTS ACCUM. kDfl	CASH FLOW ANN. kDfl	CASH FLOW ACCUM. kDfl	**NFV** kDfl	DISC. FACT. @ **228.42%**	CAPIT. COSTS ACCUM. kDfl	CASH FLOW ACCUM. kDfl	**NPV** kDfl
1	5,197	**5,197**			-5,197	1.000	**5,197**	5,197	(5,197)
2			11,870	11,870	6,674	0.304		3,614	(1,582)
3			11,870	23,741	18,544	0.093		4,715	(482)
4			11,870	35,611	30,414	0.028		5,050	(147)
5			11,870	47,481	42,285	0.009		5,152	(45)
6			11,870	59,351	54,155	0.003		5,183	(14)
7			11,870	71,222	66,025	0.001		5,193	(4)
8			11,870	83,092	77,895	0.000		5,195	(1)
9			11,870	94,962	89,766	0.000		5,196	(0)
10			11,870	106,833	101,636	0.000		5,197	(0)
11			11,870	118,703	113,506	0.000		5,197	0
ACCUM.		**5,197**		**118,703**	**113,506**	1.438	**5,197**	**5,197**	**0**

RATIO **:** [Cash Flow / Capital] @ Disc. **1.0**
NET PRESENT VALUE : [Cash Flow - Capital] @ Disc. **0**

N.B. :
1. Cash-Flows "Before Tax".
2. Earning Power = Interest, for which [Cash Flow - Capital]@Disc. = 0
   Disc. Factor = $1/(1 + r)^n$ with r = interest fraction
3. Rest Value = 6.0% of Capital Investment

When interest is 228.4%, the [Cash Flow – Capital] = 0
DCFROR = 228.4%