

CL306:- Process Engineering & Economics (PEE)

Project Report 2

Group 10

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Production Of Cyclohexanol

Problem statement:

Cyclohexanol is a colorless liquid, with a camphor-like odor. It has a general formula of $C_6H_{12}O$. It is mainly used as a precursor for the production of nylons and its application as a plasticizer and a solvent in various industries. It is commonly called as anol or naxol.

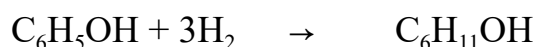
Feed
From phenol

In this process, cyclohexanol is manufactured by hydrogenation of phenol in the presence of metal catalysts such as palladium, platinum, iridium, or rubidium at a temperature of about 140 – 170°C and about atmospheric pressure.

Reactions Involved:

Reactor conversion 40%

Main Reaction:



Product:

Usually, for a commercial plant, the conversion is anywhere between 35 – 42% and the yield is in the range of 60 – 80% of the product.

Production of 100 tones/day of cyclohexanol.

Introduction & Properties

- ❖ Cyclohexanol is used in many industries as raw material and many more. Cyclohexanol is a key raw material in the preparation of a variety of high-value fine chemicals, such as polyamide 6 and polyamide 66.
- ❖ Phenol hydrogenation has two advantages: one is the low energy consumption and relatively mild reaction conditions due to the relatively low reaction temperature; the other is low contaminated and

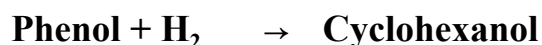
environment-friendly considering phenol is one of the important by-products or pollutants in petrochemical production and coal chemical industry.

- ❖ Palladium Phosphides have been reported to have excellent performance in the selective hydrogenation from alkynes to alkenes.
- ❖ Catalytic hydrogenation of phenol to cyclohexanone and cyclohexanol has the advantages of simple methods and environmental friendliness.
- ❖ The thermodynamics of phenol gas-phase hydrogenation reaction systems in the temperature range 400-600 K, atmospheric pressure, and hydrogen-phenol ratio in the range of 4.0-7.0.

Theory

Production Of Cyclohexanol

We can produce cyclohexanol by many reactions but here we are using the hydrogenation of phenol reaction for cyclohexanol production. The reaction is as follows.

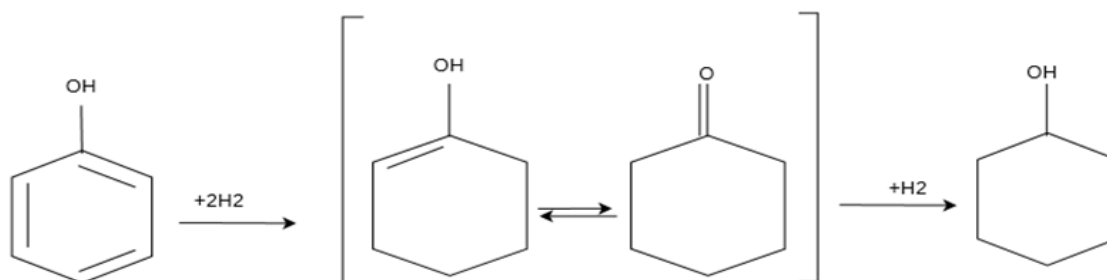


This is a heterogeneous reaction that takes place in the atmosphere. The reaction of the hydrogenation of phenol is an exothermic reaction in nature. We are using 100% pure phenol and industrial hydrogen gas as the raw material. Excess hydrogen should be ensured at the reactor's entry. A molar ratio of hydrogen to phenol should be maintained between 4.0 to 7.0. For this reaction system, some conditions are in favor to improve the conversion of phenol and the selectivity of cyclohexanol in the product which are low temperature, high pressure, and high H_2 /phenol molar ratio.

The optimum thermodynamic conditions for hydrogenation of phenol to cyclohexanol are as follows: reaction temperature is 400-600 K, the reaction pressure is 3.0-7.0 MPa, and the molar ratio of hydrogen to phenol is 4.0-7.0. The reaction system of phenol hydrogenation: The reaction system determined by the reactions was considered and cyclohexanol was the target product. The reaction system includes phenol, H_2 , 1-hydroxycyclohexene, cyclohexanone, cyclohexanol.

Reaction Mechanism

According to literature reports on phenol hydrogenation, a reaction path network is shown.



In the reaction of hydrogenation of phenol, phenol has π -bond and due to less electron density of hydrogen atoms, H_2 atom directly attacks the π -bond and makes 1-hydroxycyclohexene which convert into the cyclohexanone due to resonance. Further hydrogenation of cyclohexanone gives us our product cyclohexanol.

Cyclohexanol is formed directly by hydrogenation. One-step path-way could avoid the formation of other hydrogenated intermediate products (such as cyclohexanone

and cyclohexane). Thereby leading to 99.9% selectivity of cyclohexanol in our catalyst system.

Conceptual Process Synthesis: Hierarchy of Decisions

There are two types of synthesis for any process.

1. Hierarchical approach
2. Algorithmic approach

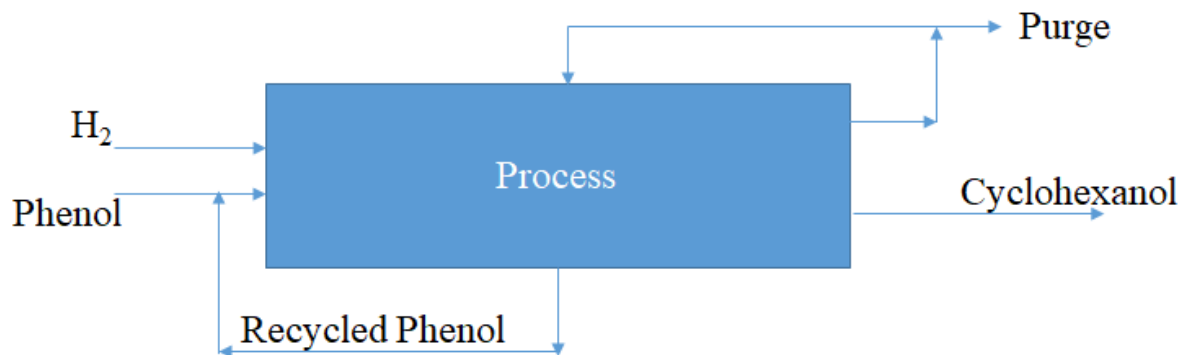
In the hierarchical approach, we will divide the design problem into several steps, develop a simple solution to these small problems and then add successive layers of detail about the design.

The process synthesis problem can be reduced to a hierarchy of designs as follows:

- Level 1 Decision: Batch V/s Continuous
- Level 2 Decision: Input-output structure of process flow sheet
- Level 3 Decision: Recycle structure of process flow sheet
- Level 4 Decision: General structure of separation system
- Level 5 Decision: Heat exchanger network

Level 1: Batch vs Continuous: Continuous process – Due to huge production of the desired product (100 tons/day)

Level 2: Input-Output Structure of the process flow-sheet



Some materials, such as air and water, are much less valuable than organic ones. Because of the low cost, the air is not normally recycled. The exit point of gases is flare.

Number of product streams leaving the process

Components	Boiling Point, $^{\circ}\text{C}$	Destination
H_2	-253	Recycle and Purge
Cyclohexanol	161.8	Primary Product
Phenol	181.7	Recycle

Though H_2 and phenol have different boiling points hence we have two recycle streams and one primary product. From one of the recycle streams, H_2 is separated as a purge. Hence the number of product streams leaving the process is Three.

Design variables

Given,

Conversion of limiting reactant (X)= 40% (35 -42 %)

Molar ratio of reactant (x)= Hydrogen/Phenol = 4.0-7.0

Reactor Temperatures= 140 °C-170 °C

With the increase of temperature, the conversions of phenol and hydrogen decrease gradually, the selectivity of cyclohexanone increases, the selectivity of cyclohexanol decreases, and the selectivity of 1-hydroxycyclohexene is zero. The hydrogenation of phenol to cyclohexanol should be carried out at a lower reaction temperature. The conversion of hydrogen increases with the increase of pressure and the decrease of the molar ratio of H_2 /phenol. With the increase of pressure and the molar ratio of H_2 /phenol, the selectivity of cyclohexanone decreases, and the selectivity of cyclohexanol increases.

Increasing the reaction pressure and H_2 /Phenol ratio leads to improved the conversion of phenol and selectivity of cyclohexanol, but the equipment cost and increase in waste lead to an increase in capital cost. Therefore the appropriate reaction pressure and H_2 /phenol ratio for phenol hydrogenation to cyclohexanol are 3.0-7.0 MPa and 4.0-7.0 respectively.

Material Balance

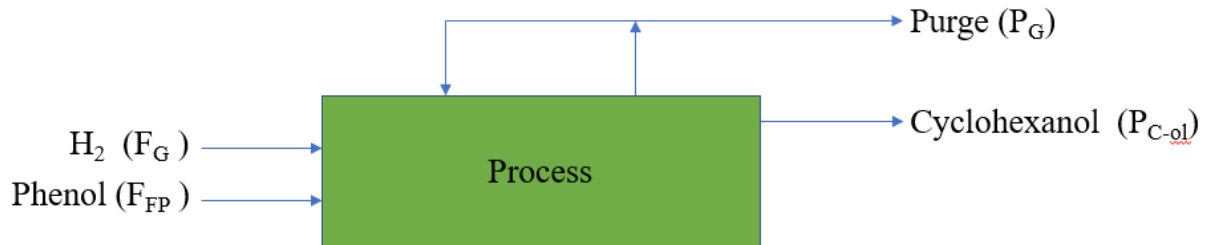
We assume a 40% conversion of phenol.

Also, per pass conversion = 40%.

No rule of thumb is available to fix the design variables. It is important to find the neighborhood of the optimum values of the design variables.

$$\text{Production rate} = 100 \text{ tones/day} = \frac{100 \text{ tones}}{M} = 10^6 \text{ moles}$$

According to stoichiometry for one mole of phenol one mole of cyclohexanol is produced. Selectivity and reaction stoichiometry.



Variables

F_{FP} = fresh pure phenol fed to process, mole/day

F_G = make-up gas stream flow rate, moles/day

P_G = flow rate of the purge stream

P_{C-ol} = desired cyclohexanol production, 10^6 moles/day

P_{RP} = flow rate of recycled phenol, mole/day

$$\diamond \text{ Conversion}(X) = \frac{\text{Reactant consumed in the reactor}}{\text{Reactant fed to the reactor}} = 40 \% = 0.4$$

$$\diamond \text{ Selectivity}(S) = \frac{\text{Desired product produced}}{\text{Reactant fed to the reactor}} * (SF)$$

H₂ Balance:

The total amount of hydrogen fed to the process will be = net H₂ consumed
+ H₂ lost in the purge

$$F_G = P_G + PRG \quad \dots\dots\dots(1)$$

Phenol Balance:

$$FFP + PRP = PC_{-ol} \quad \dots\dots\dots(2)$$

Required product flow rate (p_{C-ol}) = 100 tones/day

According to the stoichiometry of the reaction

For 1 mole of phenol 1 mole of cyclohexanol will form and 3 moles of hydrogen will be consumed.

Hence,

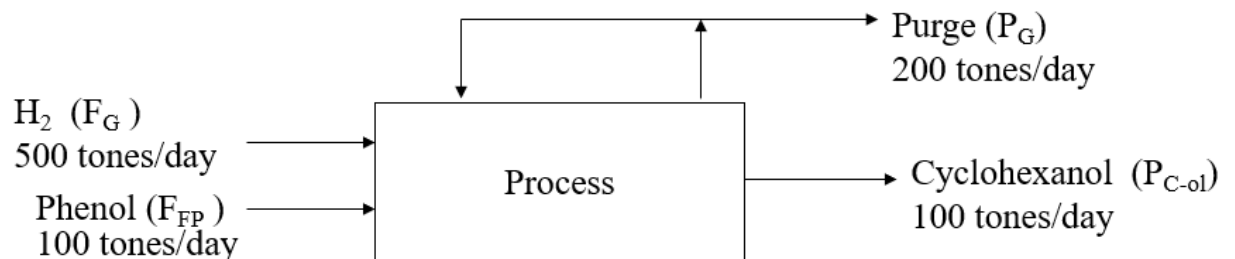
Flow rate of raw material, $F_{FP} = 100$ tones/day

And, Hydrogen/ phenol = 5 (Assumed)

Hydrogen fed to the process = $100 * 5 = 500$ tones/day

Hydrogen consumed in the process = $500 - 300 = 200$ tones/day

$F_G = 500$ tones/day (excess hydrogen for complete conversion of toxic phenol)



Overall mass balance:

mass input = mass output + mass consumed in reaction

$$\text{Mass input} = 100 + 500 = 600 \text{ tones/day}$$

$$\text{Mass output} = 100 + 200 = 300 \text{ tones/day}$$

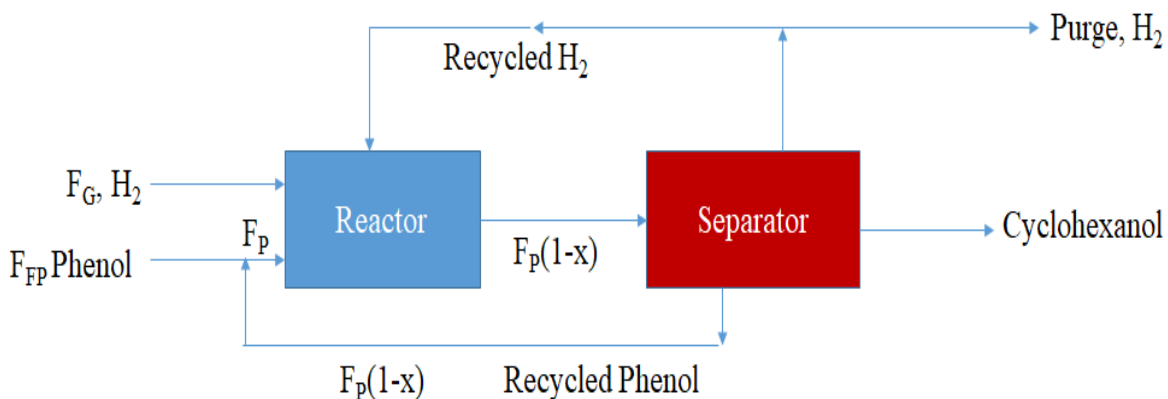
Level 3: Recycle Structure

Recycle structure depends on the following:

A single reactor system is required since temperature and pressure conditions and catalyst are the same in the whole process.

Two recycle streams are required, one for hydrogen and the other for phenol.

Amount of excess reactant. (i.e. hydrogen) Large excess implies greater selectivity and excess reactant may force one component to close to complete conversion and also shifts the equilibrium to the right-hand side.



Recycle material balance:

Per pass conversion = 40%.

Assuming 100% recovery and recycle of limiting reactant. (i.e. phenol)

Let, F_p be the flow rate of phenol entering the reactor

Let, X , be the conversion so phenol leaving the reactor = $F_p(1-X)$

Material balance at the mixing point before the reactor.

$$F_{FP} + F_p(1 - X) = F_p$$

$$F_p = F_{FP}/X$$

Product formed = 0.4 (total phenol feed to the reactor)

Total phenol fed to the reactor = $100/0.4 = 250 \text{ tones/day}$

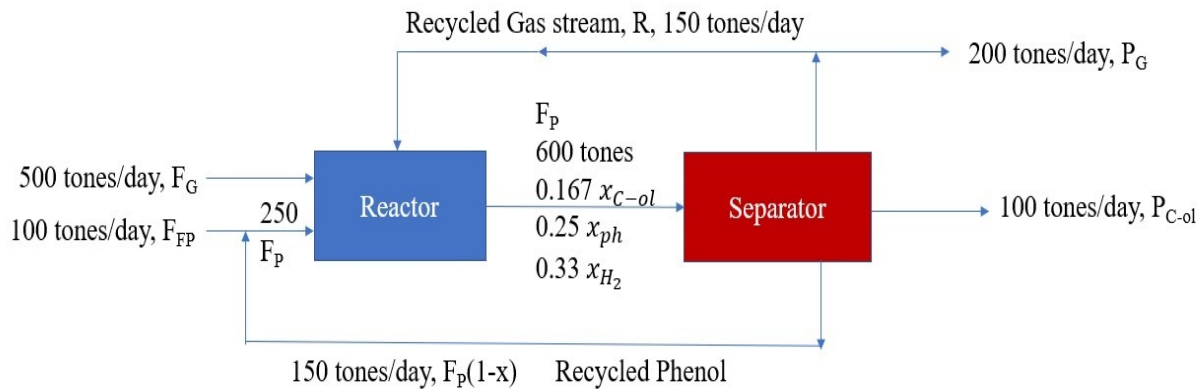
Fresh phenol feed = 100 tones/day

Recycled phenol = $250 - 100 = 150 \text{ tones/day}$

Hydrogen gas consumed in the reaction = $100 * 3 = 300 \text{ tones/day}$

Hydrogen in purge stream = $500 - 300 = 200 \text{ tones/day}$

Recycled gas stream = $600 - 150 - 100 - 200 = 150 \text{ tones/day}$



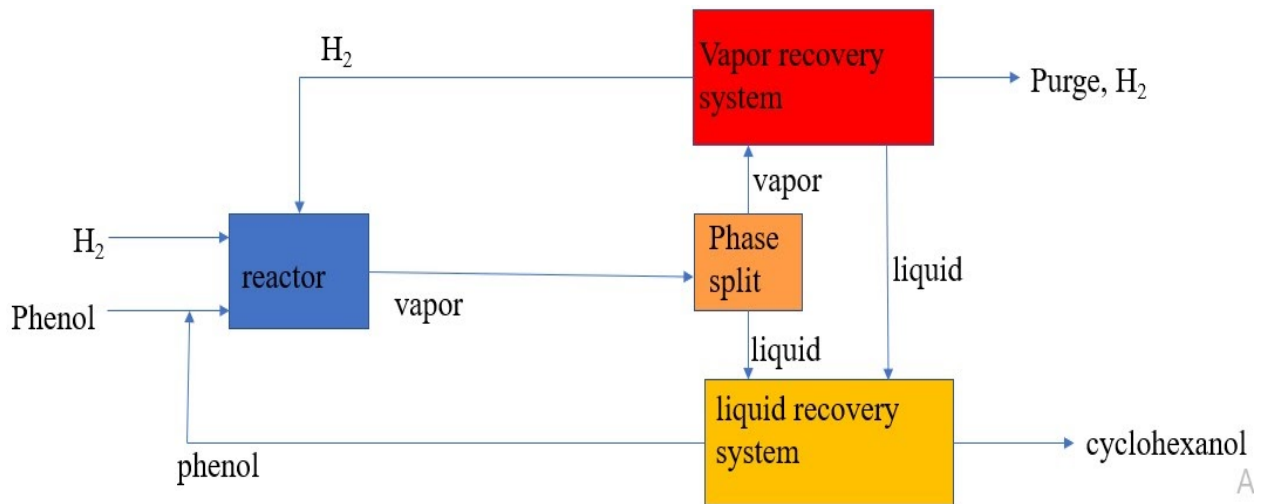
Level 4: Synthesis of the separation system

We assume vapor phase reactor effluent in the process.

We are required to cool the vapor stream to 35 °C, then completely condense the vapor.

Then send this condensed liquid to the liquid recovery system and condensed vapor to the vapor recovery system.

The separation process can also be done by phase split since this is the cheapest method of separation.



Energy Balance

1. FEHE (mixing point of phenol and recycled phenol)

Fresh phenol and recycled phenol are mixed here and sent to the evaporator.

I/P: Phenol (x) @ 75 °C, 100tones/day = 44.27kmol/hr

Recycled phenol (R) @ 145 °C, 150tones/day = 66.41kmol/hr

O/P : Phenol (x+R) @ 93 °C, 250tones/day = 110.68kmol/hr

stream	T	specific heat	flow rate	heat
x	75	185.3	44.27	615242.325
R	145	238.2	66.41	2293734.99
x+R	93	191.8	110.68	1974243.432

Heat in = 2908976.325 KJ/hr

Heat out = 1974243.42 KJ/hr

Heat of mixing = heat in - heat out = 934733.883 KJ/hr

2. Plug Flow Reactor

Here, Reaction takes place and the product is formed which is sent to the separator.

I/P: Phenol (x+R) @ 93°C, 250 tones/day = 110.68 kmol/hr

H₂ (gas) → 500 tones/day = 10416.67 kmol/hr

O/P: 0.6(x+R) phenol @160 °C

Y₁ H₂ gas = 200 tones/day = 4166.67 kmol/hr

0.4(x+R) cyclohexanol

Input stream flow rate = 110.68 + 10416.67 = 10527.35 kmol/hr

Output stream flow rate = 4166.67 + 110.68 = 4277.35 kmol/hr

Heat of reaction = -1630.74 KJ/hr

stream	T	specific heat	flow rate	heat
input	93	191.8	10527.35	187780552.9
output	160	162.1	4277.35	110937349.6

Heat required = heat out - heat in + heat of reaction

$$= 110937349.6 - 187780552.9 + (-1630.74)$$

Heat required = 76844834.03 KJ/hr

3. Distillation column

I/P: @ 79 °C 0.6(x+R) phenol

@ 79 °C 0.4(x+R) cyclohexanol

O/P: @ 145 °C phenol (R)

@ 161.8 °C Cyclohexanol (x)

stream	T	specific heat	flow rate	heat
input	79	132.8	110.68	1161166.016
phenol	145	238.2	66.41	2293734.99
cyclohexanol	161.8	198.27	44.27	1420185.407

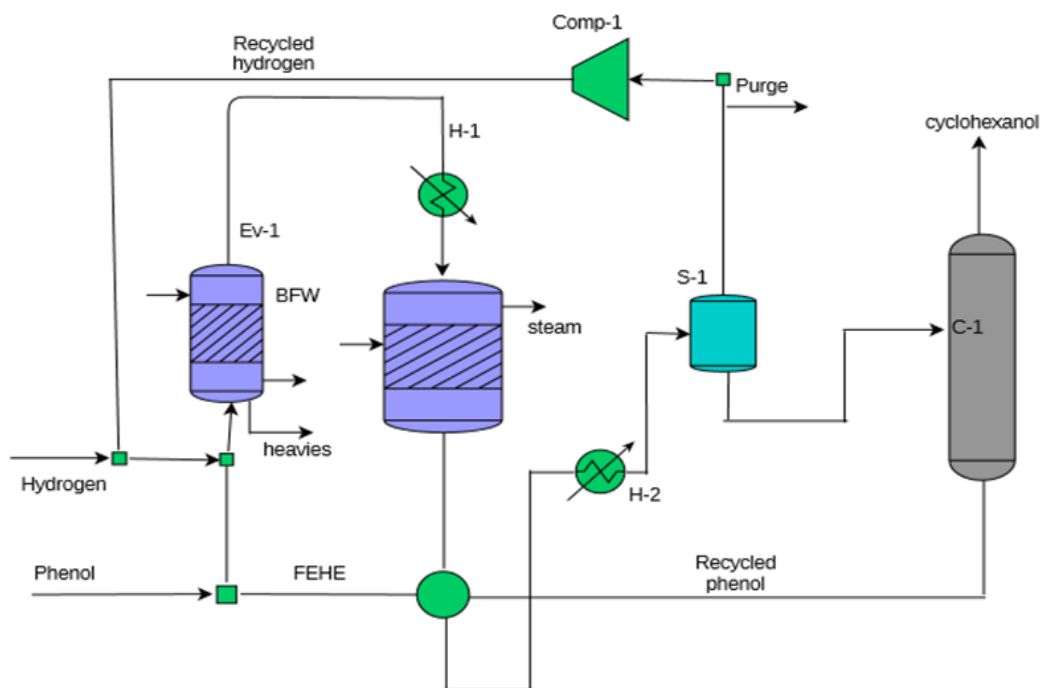
Heat in = 1161166.016 KJ/hr

Heat out = 3713920.397 KJ/hr

Heat required = heat out - heat in = 2552754.381 KJ/hr

Process flow sheet

The final flowsheet is drawn after all the levels of the hierarchy of decisions



ECONOMIC POTENTIAL

For level 2:

Economic Potential = Value of Products and Byproducts – Cost of Raw Materials

Raw Materials:

Cost of phenol = (Rs. 107407.85/ton)*100tones/day

$$= \text{Rs. } 10740785/\text{day}$$

Cost of H₂ = Rs. 0.00 (use as fuel gas) {Cost of handling = fuel gas credit}

Products:

Cost of cyclohexanol = (Rs. 190000/ton)*100tones/day

$$= \text{Rs. } 19000000$$

EP₂ = Value of Products – Cost of Raw Materials

$$= 19000000 - 10740785$$

$$= \text{Rs. } 8259215/\text{day}$$

For level 3:

EP₃ = EP₂ - compressor/pump - reactor costs(PFR)

Cost of PFR = Rs. 2000000/- (Weihai Zhengwei Machinery Co., Ltd.)

Cost of compressor = Rs. 500000/- (Indiamart, Mumbai, Maharashtra)

$$\text{EP}_3 = \text{Rs. } (8259215 - 2000000 - 500000)$$

$$\text{EP}_3 = \text{Rs. } 5759215/-$$

For level 4:

$$EP_4 = EP_3 - \text{cost of separation} - \text{utility cost} - \text{additional environmental cost}$$

Cost of Components:

Distillation column = Rs.1000000/- (Excel Plants & Equipment Pvt Ltd, Pune)

Reboiler = Rs. 100000/- (Ascent Machineries & Engg. Services)

Condenser = Rs. 75000/-

Reflux drum = Rs. 850000/- (Kalina Engineering Pvt Ltd, Bhayandar East, Mumbai)

$$EP_4 = 575215 - (1000000 + 100000 + 75000 + 850000) - 0$$

$$EP_4 = \text{Rs. } 1449785/-$$

Heat exchanger Design

In intercoolers, boilers, pre-heaters, and condensers inside power plants as well as other engineering processes, heat exchangers are utilized for controlling heat energy. Heat exchangers are devices that regulate efficient heat transfer from one fluid to another.

The optimum thermal design of a shell and tube heat exchanger involves the consideration of many interacting design parameters which can be summarized as follows:

Process:

1. Process fluid assignments to shell side or tube side.

2. Selection of stream temperature specifications.
3. Setting shell side and tube side pressure drop design limits.
4. Setting shell side and tube side velocity limits.
5. Selection of heat transfer models and fouling coefficients for shell side and tube side.

Mechanical:

1. Selection of heat exchanger TEMA layout and number of passes.
2. Specification of tube parameters - size, layout, pitch and material.
3. Setting upper and lower design limits on tube length.
4. Specification of shell side parameters – materials, baffles cut, baffle spacing and clearances.
5. Setting upper and lower design limits on shell diameter, baffle cut and baffle spacing.

The Heat Exchanger calculations:

Basic heat exchanger equation is:

$$Q = U * A * \Delta T_m$$

The log mean temperature difference ΔT_m is:

$$\Delta T_m = \frac{(T_1 - t_2) - (T_2 - t_1)}{\ln \frac{(T_1 - t_2)}{(T_2 - t_1)}}$$

The amount of heat required to raise the temperature of a substance can be expressed as:

$$Q = m.c_p.dT$$

Where,

Q = Quantity of energy or heat (kJ) (Btu);

m = Mass of the substance (kg) (lb);

c_p = Specific heat capacity of the substance (kJ/kg °C) or (Btu/(lb.°F));

dT = Temperature rise of the substance (°C) (°F);

U = Overall heat transfer coefficient;

T_1 = Inlet tube side fluid temperature;

T_2 = Outlet tube side fluid temperature;

t_1 = Inlet shell side fluid temperature.

t_2 = Outlet shell side fluid temperature;

The overall design process:

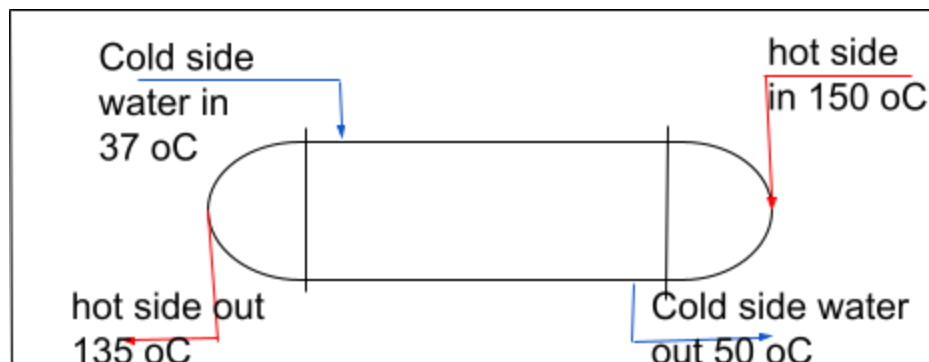
Here is a set of steps for the process. Design of a heat exchanger is an iterative (trial & error) process:

- Calculate the required heat transfer rate, Q , in Btu/hr from specified information about fluid flow rates and temperatures.
- Make an initial estimate of the overall heat transfer coefficient, U , based on the fluids involved.
- Calculate the log mean temperature difference, ΔT_m , from the inlet and outlet temperatures of the two fluids.
- Calculate the estimated heat transfer area required, using: $A = Q/(U \Delta T_m)$. Select a preliminary heat exchanger configuration.
- Make a more detailed estimate of the overall heat transfer coefficient, U , based on the preliminary heat exchanger configuration.
- Estimate the pressure drop across the heat exchanger. If it is too high, revise the heat exchanger configuration until the pressure drop is acceptable.

- If the new estimate of U is different from the previous estimate, repeat steps 4 through 7 as many times as necessary until the two estimates are the same to the desired degree of accuracy.
- Input information needed. In order to start the heat exchanger design process, several items of information are needed as follows:
 - ❖ The two fluids involved need to be identified;
 - ❖ The heat capacity of each fluid is needed;
 - ❖ The required initial and final temperatures for one of the fluids are needed;
 - ❖ The design value of the initial temperature for the other fluid is needed;
 - ❖ An initial estimate for the value of the **Overall Heat Transfer Coefficient, U** , is needed.

Note: In calculation, knowing the first four items allows determination of the required heat transfer rate, Q , and the inlet and outlet temperatures of both fluids, thus allowing calculation of the log mean temperature difference, ΔT_m . With values now available for Q , U , and ΔT_m , an initial estimate for the required heat transfer area can be calculated from the equation:

$$A = Q / (U \cdot \Delta T_m)$$



Sample Calculations

Let mass flow rate to the heat exchanger, $m = 10.417 \text{ g/hr} = 63775.51 \text{ mole/hr}$

Specific heat of phenol at ambient condition, $c_p = 145.52 \text{ J/mole.K}$

$T_1 = 150^\circ\text{C} = 423.15 \text{ K}$; $T_2 = 135^\circ\text{C} = 408.15 \text{ K}$;

$t_1 = 37^\circ\text{C} = 310.15 \text{ K}$; $t_2 = 50^\circ\text{C} = 323.15 \text{ K}$;

$$Q = 63775.51 * 145.52 * (423.15 - 408.15) = 139209183.7 \text{ J/hr}$$

$$\Delta T_m = \frac{(423.15-323.15)-(408.15-310.15)}{\ln \frac{(423.15-323.15)}{(408.15-310.15)}} = 98.99 \text{ K}$$

Assumed, $U = 120 \text{ Btu/hr.ft}^2.\text{°F} = 681.42 \text{ W/m}^2.\text{K}$

Area estimate of heat exchanger:

$$A = 139209183.7 / (681.42 * 98.99) = 2063.772 \text{ m}^2$$

Required mass flow rate of water:

$$c_p = 75.3 \text{ J/mol.K (@ } T = 43.5^\circ\text{C} = (t_1+t_2)/2)$$

$$m = Q/c_p.\Delta T_m = 139209183.7/75.3*98.99 = 18675.9 \text{ mol/hr}$$

No. of tubes calculation:

Let for the tube of $D = 3 \text{ m}$ diameter and $L = 10 \text{ m}^2$ length

Surface area of heat transfer, $S = \pi DL = \pi*3*10 = 94.25 \text{ m}^2$

No. of tubes required = $2063.772/94.25 = 22$

Following is a table with values for different applications and heat exchanger types:

Typical Overall Heat Transfer Coefficients in Heat Exchangers			
Type	Application and Conditions	U	U
		W/(m².K)	Btu/(hr.ft².°F)
Tubular, heating or cooling	Gases at atmospheric pressure inside and outside tubes	5 - 35	1 - 6
	Gases at high pressure inside and outside tubes	150 - 500	25 - 90
	Liquid outside (inside) and gas at atmospheric pressure inside (outside) tubes	15 - 70	3 - 15
	Gas at high pressure inside and liquid outside tubes	200 - 400	35 - 70
	Liquids inside and outside tubes	150 - 1200	25 - 200
	Steam outside and liquid inside tubes	300 - 1200	50 - 200
Tubular, condensation	Steam outside and cooling water inside tubes	1500 - 4000	250 - 700
	Organic vapors or ammonia outside and cooling water inside tubes	300 - 1200	50 - 200
Tubular, evaporation	Steam outside and high-viscous liquid inside tubes, natural circulation	300 - 900	50 - 150
	Steam outside and low-viscous liquid inside tubes, natural circulation	600 - 1700	100 - 300
	Steam outside and liquid inside tubes, forced circulation	900 - 3000	150 - 500
Air-cooled heat exchangers	Cooling of water	600 - 750	100 - 130
	Cooling of liquid light hydrocarbons	400 - 550	70 - 95
	Cooling of tar	30 - 60	5 - 10
	Cooling of air or flue gas	60 - 180	10 - 30
	Cooling of hydrocarbon gas	200 - 450	35 - 80
	Condensation of low pressure steam	700 - 850	125 - 150
	Condensation of organic vapors	350 - 500	65 - 90
Plate heat exchanger	Liquid to liquid	1000 - 4000	150 - 700
Spiral heat exchanger	Liquid to liquid	700 - 2500	125 - 500
	Condensing vapor to liquid	900 - 3500	150 - 700

DISTILLATION COLUMNS:NUMBER OF TRAYS

Overhead and Bottom Compositions

For preliminary designs, we use the rule of thumb that we desire 99.5% recoveries of the light key in the overhead and 99.5% of the heavy key are taken overhead and that all components heavier than the heavy key leave with the bottoms.

Column Pressure

The operating pressure for a distillation column normally is fixed by the economic

Desirability of using a condenser supplied with cooling towers. We want to ensure that the condenser will be sufficiently large to condense that vapors even on hot days, so we assume that cooling water is available at 90 °F. Also, the design of the cooling towers is based on the assumption that all that streams returned the tower have temperatures of 120 oF or less, because the scaling and corrosive characteristics of water become very pronounced above that temperature (i.e., calcium and magnesium salts are deposited on the exchanger walls.

In cases where the overhead bubble point exceeds 267 °F, we operate the condenser at atmospheric pressure, but we generate steam instead of using cooling water.

Estimating Bubble Points and Dew Points

For most hydrocarbon mixtures (those do not exhibit hydrogen bonding) we write the equilibrium expression as

$$y_i = K_i * x_i$$

$$y_i = \frac{K_i x_i}{\sum K_i x_i}$$

$$\phi_i = \frac{K_i}{K_{HK}}$$

$$y_i = \phi_i x_i / \sum \phi_i x_i$$

Bubble Points

$$y_i/x_i = \phi_i / \sum \phi_i x_i = K_i$$

Then use the value of the K correlations, to find the temperature at the specified column pressure. Normally, we calculate the K value for the light key to estimate the temperature.

Dew Point

$$y_i/x_i = (1/x_i) / \sum y_i / \phi_i = K_i$$

Once we estimate K for the light key, we use a correlation to find the temperature.

Relative Volatility

The constant value of ϕ_i used in these calculations is normally taken to be the geometric mean of the top and bottom values:

$$\phi_{i,av} = \sqrt{\phi_{i,top} \phi_{i,bottom}}$$

Whenever the boiling points of the overhead and bottom product are widely separated, α_{top} is often much greater than α_{bottom} . The assumption of constant α is not valid for the systems, and the assumption of constant molar overflow is not usually valid.

Estimating the Number of Theoretical Trays for Sharp Splits in Simple in Simple Columns

GILLILAND'S CORRELATION.

$$\frac{N-N_m}{N+1} = 0.75 \left[1 - \left(\frac{R-R_m}{R+1} \right)^{0.5688} \right]$$

We can calculate N after we have estimated N_m (minimum number tray at total reflux), R_m (minimum reflux ratio), R (actual reflux ratio)

FENSKE'S EQUATION FOR THE MINIMUM TRAYS AT TOTAL REFLUX N_m .

$$N_m = \frac{\ln SF}{\ln \alpha_{av}}$$

Separation factor(SF)

$$SF = \frac{x_D (1-x_W)}{x_W (1-x_D)}$$

Where,

D - Distillate; W- Bottom

UNDERWOOD'S EQUATION FOR THE MINIMUM REFLUX RATIO R_m .

For a binary system with constant α , the minimum reflux ratio corresponds to the common intersection of the operating line in the rectifying section of the tower

$$y = \frac{R_m}{R_m+1}x + \frac{x_D}{R_m+1}$$

The equilibrium curve

$$y = \frac{\alpha x}{1 + (\alpha - 1)x}$$

And the q line representing the feed quality

$$y = \frac{q}{q-1}x - \frac{z_F}{q-1}$$

Where q is the heat required to vaporize 1 mol of feed divided by the heat of vaporization.

For the case of saturated-liquid feed where $q=1$,

$$R_m = \left(\frac{1}{\alpha - 1} \right) \left[\frac{x_D}{x_F} - \frac{\alpha(1-x_D)}{1-x_D} \right]$$

Similarly, for saturated-vapor feed where $q=0$,

$$R_m = \left(\frac{1}{\alpha - 1} \right) \left[\frac{\alpha x_D}{y_F} - \frac{(1-x_D)}{1-y_F} \right] - 1$$

OPERATING REFLUX RATIO R .

As the reflux ratio is increased above the minimum, the number of trays required for a given separation decreases, so that the capital cost of the column decreases. However, increasing the reflux ratio will increase the vapor rate in the tower, and, as we show later, higher vapor rates correspond to more expensive condensers and reboilers, along with higher cooling-water and steam costs. Therefore, there is an optimum reflux ratio for any specified separation.

Rule of thumb:

The operating reflux ratio is chosen so that $R/R_m = 1.2$

SIMPLIFIED APPROXIMATION OF GILLILAND'S CORRELATION.

$$N \sim 2N_m = 2 \frac{\ln SF}{\ln \alpha}$$

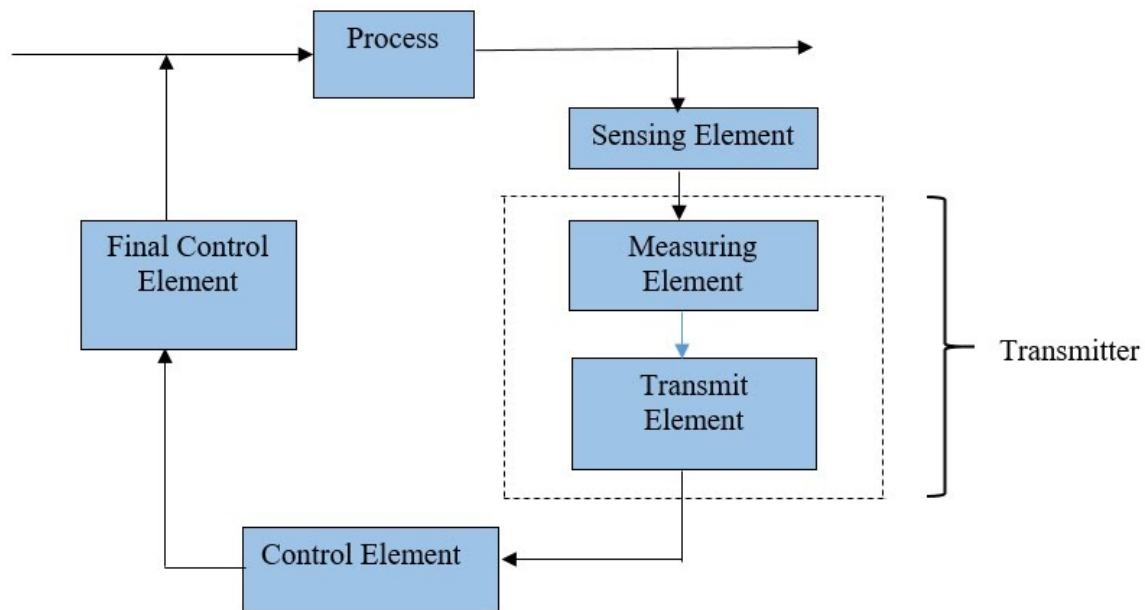
Instrumentation and Control for the Equipments

PID FEEDBACK CONTROL SYSTEM

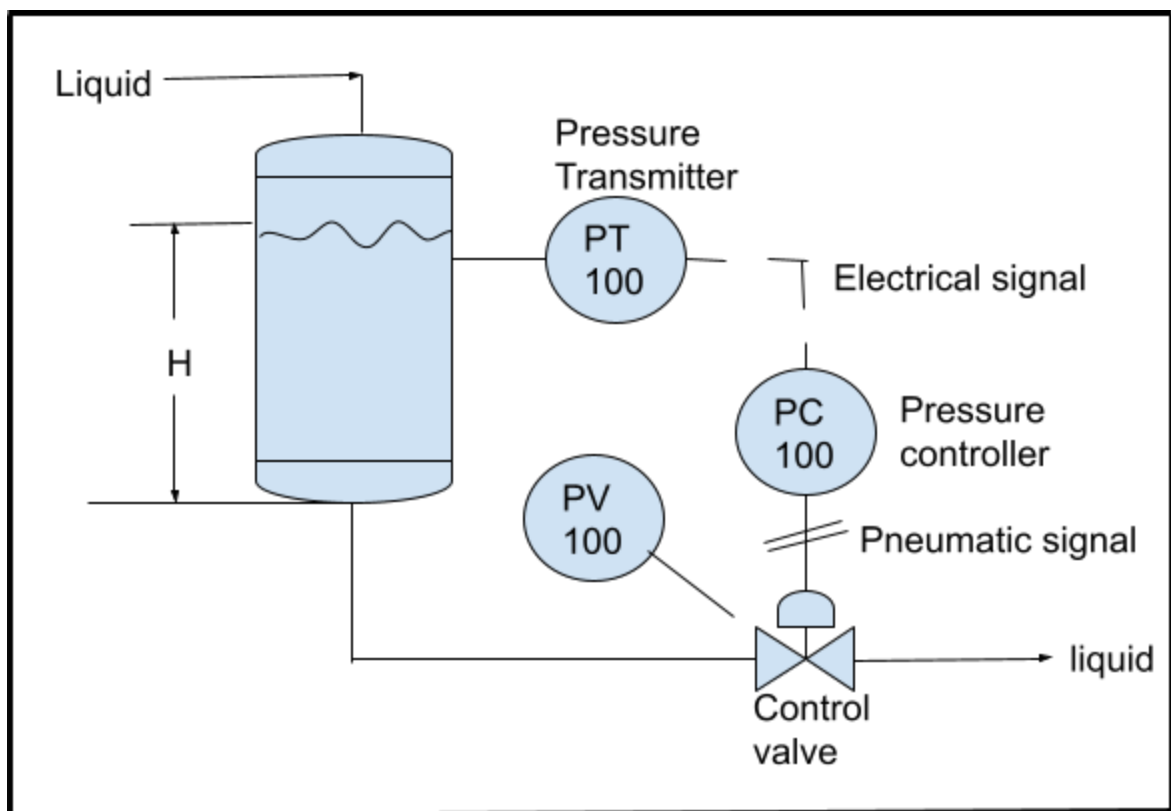
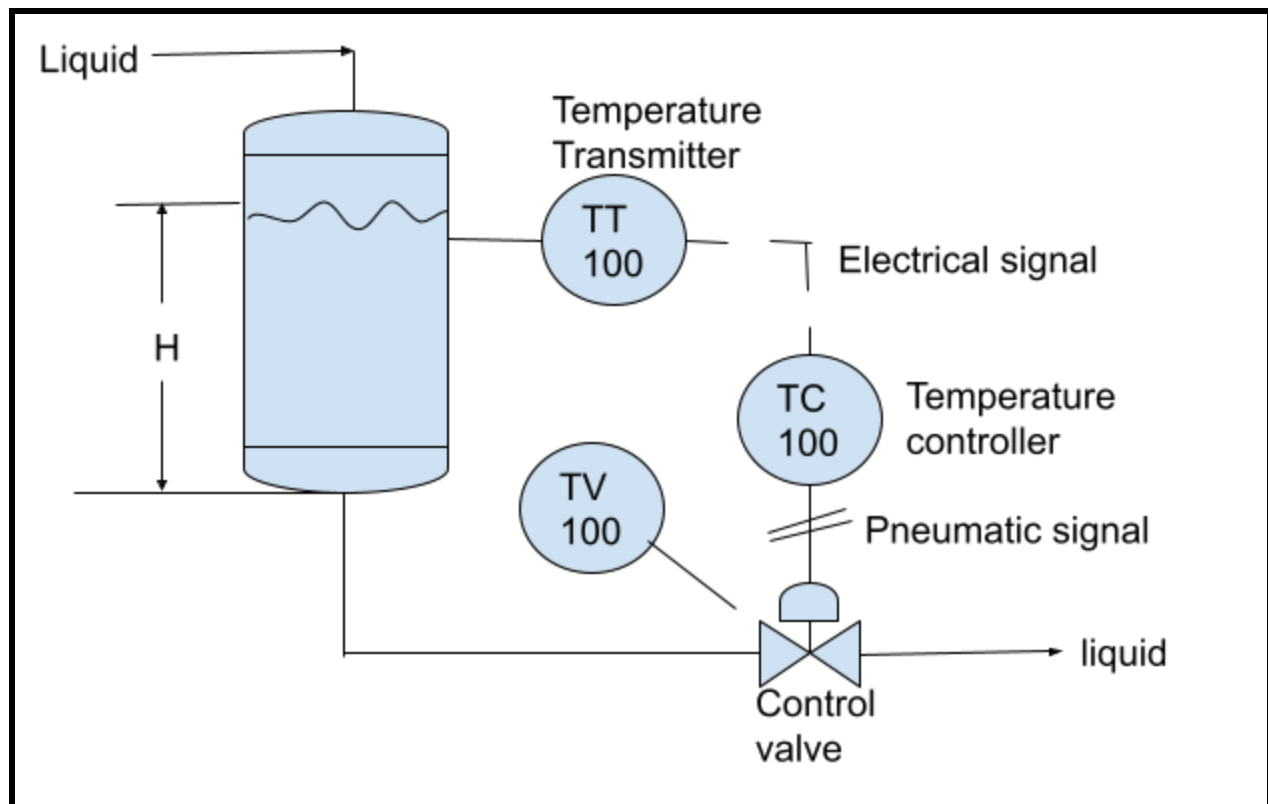
Reaction conditions of the reactor (Tubular reactor) should be low temp and around atmospheric pressure. So we cannot expect a higher increase in temp and

much lower and higher pressure. We need a control system for the reactor. Using a PID feedback control system is the best option that we have.

Schematic for the reactor control system:



Like a feedback control system, we can have a feedforward control system. Which will be used as per our requirement. Incase inlet flow rate to system has no influence in system mixture/ outlet stream due to large volume of system in that case we can use feedforward system. The three parameters are most important for the whole process for the safety factor of the environment. We can have control for temperature, pressure, liquid level, composition in different systems like reactor, mixer, heat exchanger etc.



SELECTION OF EQUIPMENTS

1. PFR Reactor:



The plug flow reactor model (PFR, sometimes called continuous tubular reactor, CTR) is normally the name given to a model used in chemical engineering to describe chemical reactions in continuous, flowing systems of cylindrical geometry.

Working pressure: Negative pressure: -0.1~9.8 MPa

Working Temperature: -196~350 °C

2. Distillation Column:



Distillation columns (distillation towers) are made up of several components, each of which is used either to transfer heat energy or enhance material transfer. A typical distillation column consists of several major parts:

- a) vertical shell where separation of the components is carried out.
- b) Column internals such as trays, or plates, or packings are used to enhance component separation.
- c) A reboiler to provide the necessary vaporization for the distillation process.

- d) A condenser to cool and condense the vapor leaving the top of the column.
- e) A reflux drum holds the condensed vapor from the top of the column so that liquid (reflux) can be recycled back to the column.

3. Reflux Drum:

Part of Condensate collected from the condenser will be collected in the reflux drum. And will be returned to the upper part of the distillation column. Inside the column, the down-flowing reflux liquid provides cooling and condensation of the up-flowing vapors thereby increasing the efficiency of the distillation tower.



4. Reboiler:

Reboilers are heat exchangers typically used to provide heat to the bottom of industrial distillation columns. They boil the liquid from the bottom of a distillation column to generate vapors which are returned to the column to drive the distillation separation. The heat supplied to the column by the reboiler at the bottom of the column is removed by the condenser at the top of the column.



5. Condenser:

Condenser, a device for reducing a gas or vapor to a liquid. Condensers are employed in power plants to condense exhaust steam from turbines and in refrigeration plants to condense refrigerant vapors, such as ammonia and fluorinated hydrocarbons. The petroleum and chemical industries employ condensers for the condensation of hydrocarbons and other chemical vapors. In distilling operations, the device in which the vapor is transformed to a liquid state is called a condenser.

Flow rate: up to 50m³

Working Pressure: max. 10Mpa



6. Compressor:

A compressor is a mechanical device that increases the pressure of a gas by reducing its volume. Compressors are similar to pumps i.e. both increase the pressure on a fluid and both can transport the fluid through the pipe.



7. Evaporator:

An evaporator is a device in a process used to turn the liquid form of a chemical substance such as water into its gaseous form/vapor. The liquid is evaporated or vaporized, into a gas form of the targeted substance in that process.



Total capital investment and total cost estimation

Capital investment : classification

Total capital investment (TCI)= fixed capital investment (FCI) + working Capital (WC)

Fixed Capital Investment:

Cost of equipment and facilities $FCI = (\text{Direct Costs}) + (\text{Indirect Costs})$

Direct Costs:

1. Purchased equipment: Columns, Heat Exchangers, pumps, tanks, etc.
2. Equipment Installation
3. Piping (includes insulation)
4. Instruments and Control
5. Electrical Equipment.
6. Buildings: Process, Administration, Maintenance shops, etc.
7. Site Preparation
8. Service Facilities: steam, water, air, fuel, etc. Waste treatment, fire control, offices, etc.
9. Land

Indirect Costs:

1. Engineering and Supervision: Administrative and Design. Supervision and Inspection.
2. Construction Expenses
3. Contractor's fee
4. Contingency.
5. Start-up expenses

Cash flow for industrial operation:

Net cash flow from the project = (total income from sales (S) - cost for operation(C) - depreciation(D)) (1 - income tax(θ)) + D

Estimation of capital investment:

Cost indexes:

Many different types of cost indexes are published regularly. Some of these can be used for:

- Estimating equipment costs
- Labor cost
- Construction and materials cost
- or other specialized fields.

The most common cost indexes are:

- Marshall and Swift equipment cost index
- Engineering News Record construction index
- Nelson Farrar refinery construction index
- Chemical Engineering plant cost index

$$Present\ Cost = (original\ cost\ at\ time\ t) * \left(\frac{index\ value\ now}{index\ value\ at\ time\ t} \right)$$

Estimating equipment cost by scaling:

- Mostly cost data for the desired size or capacity may not be available
- Predictions can be made by using power relationship known as six tenth factor rule (if new equipment is similar but of different capacity than the one in available data)

$$cost\ of\ equipment\ of\ capacity\ c_1 = cost\ equipment\ capacity\ c_2 * \left(\frac{c_1}{c_2} \right)^{0.6}$$

Methods of Estimating Capital investment:

1. DETAILED ITEM ESTIMATE: (used for detailed)

- Cost data of equipments and materials

Components	Cost
FEHE	₹ 1,00,000
Reactor	₹ 20,00,000
Evaporator	₹ 2,00,000
Flash Drum	₹ 8,96,814
Distillation Column	₹ 10,00,000
Reflux Drum	₹ 8,50,000
Reboiler	₹ 1,00,000
Condenser	₹ 75,000
Compressor	₹ 5,00,000
Pump	₹ 75,900
Valve	₹ 36,000
Pipes	₹ 10,00,000
Total Component Cost	₹ 68,32,900

- Estimation of installation cost:
 - Accurate labor cost
 - Efficiencies
 - Employee-hour calculation
- Accurate estimates of engineering, drafting, field supervision, employee-hour and field expenses.

2. PERCENTAGE OF DELIVERED EQUIPMENT COST:

This method for estimating the fixed or total capital investment requires:

- Determination of the delivered equipment cost.
- The other items included in the total direct plant cost are then estimated as percentages of the delivered equipment cost.
- The additional components of the capital investment are based on average percentages of the total direct plant cost, total direct and indirect plant costs, or total capital investment.

$$C_n = \Sigma E + f_1 E + f_2 E + \dots + f_n E = E \Sigma (1 + f_1 + f_2 + \dots + f_n)$$

Where

f_1, f_2, \dots, f_n = multiplying factors for piping, electrical, instrumentation, indirect costs

Equipment Cost, E = ₹ 68.329 lakh

Ratio factors for estimating capital-investment items based on delivered equipment cost				
Item	Percent of delivered equipment cost for			
	Solid processing, f_1	Solid-fluid, f_2	Fluid processing, f_3	Cost, $f_2 * E * 10^5$
Direct cost				
Purchased equipment-delivered	100	100	100	68.329

Purchased-equipment installation	45	39	47	26.648
Instrumentation and controls (installed)	18	26	36	17.766
Piping (installed)	16	31	68	21.182
Electrical (installed)	10	10	11	6.8329
Buildings (including services)	25	29	18	19.815
Yard improvements	15	12	10	8.199
Service facilities (installed)	40	55	70	37.581
Total direct plant cost D				206.353
Indirect Costs				
Engineering and supervision	33	32	33	21.865
Construction expenses	39	34	41	23.232
Contractor's fee + legal expenses	21	23	26	15.716
Contingency	35	37	44	25.282
Total indirect plant cost				86.095
Working capital (about 15% of total capital investment)	70	75	89	
Fixed Capital Investment				₹292.448

Total Capital Investment = $292.448 / 0.85 = ₹ 344.0564$ lakh

Working Capital Investment = $344.0564 * 0.15 = ₹ 51.6084$ lakh

3. “LANG” FACTORS FOR APPROXIMATION OF CAPITAL:

The cost of a process plant may be obtained by multiplying the basic equipment cost by some factor to approximate the capital investment. These values are combined to give Lang multiplication factors.

Lang multiplication factors for estimation of fixed capital investment or total capital investment:

Factor \times delivered equipment cost = fixed capital investment or total capital investment. i.e.,

$$C_n = fC$$

Lang multiplication factor:

Type of plant	Factor for investment Fixed capital	Total capital
Solid processing plant	4.0	4.7
Solid fluid processing plant	4.3	5.0
Fluid processing plant	5.0	6.0

Delivered equipment Cost = ₹68.329 lakh (Assumed)

Total fixed investment = $4.3 * 68.329 = ₹ 293.8147 \text{ lacs}$

Total Capital investment = $5.0 * 68.329 = ₹341.645 \text{ lacs}$

4. POWER FACTOR APPLIED TO PLANT CAPACITY RATIO:

This method for study or order of magnitude estimates relates the fixed capital investment of a new process plant to the fixed capital investment of similar previously constructed plants by an exponential power ratio.

The fixed capital investment of the new facility is:

$$C_n = C f_e R^x ; \quad R = S_n / S$$

Where,

f_e = cost index ratio

C, C_n = Fixed capital investment of old and new facility

S, S_n = Capacity of old and new facility

x = Capacity power factor

If the split of direct and indirect costs is known,

$$C_n = f(DR^x + I)$$

D, I = Direct and Indirect cost

Note: $x = 0.6$ should be taken if the capacity power factor is not given.

Fixed capital Investment, $C = ₹292.448 \text{ lakh}$

$$\frac{S_n}{S} = 3 \text{ (Assumed)}$$

$$f_e = 4.2 \text{ (Assumed)}$$

$$\text{New fixed capital investment, } C_n = 292.448 * 4.2 * 3^{0.6} = ₹ 2374.492 \text{ lakh}$$

5. TURNOVER RATIOS :

$$\frac{\text{Annual production rate} \times \text{Average selling price}}{\text{Gross annual sales}} = \text{Turnover ratio}$$

where the product of the annual production rate and the average selling price of the commodities is the gross annual sales figures.

Turnover ratio is less than 1 i.e. in We have to increase conversion of reaction. We are at a loss.

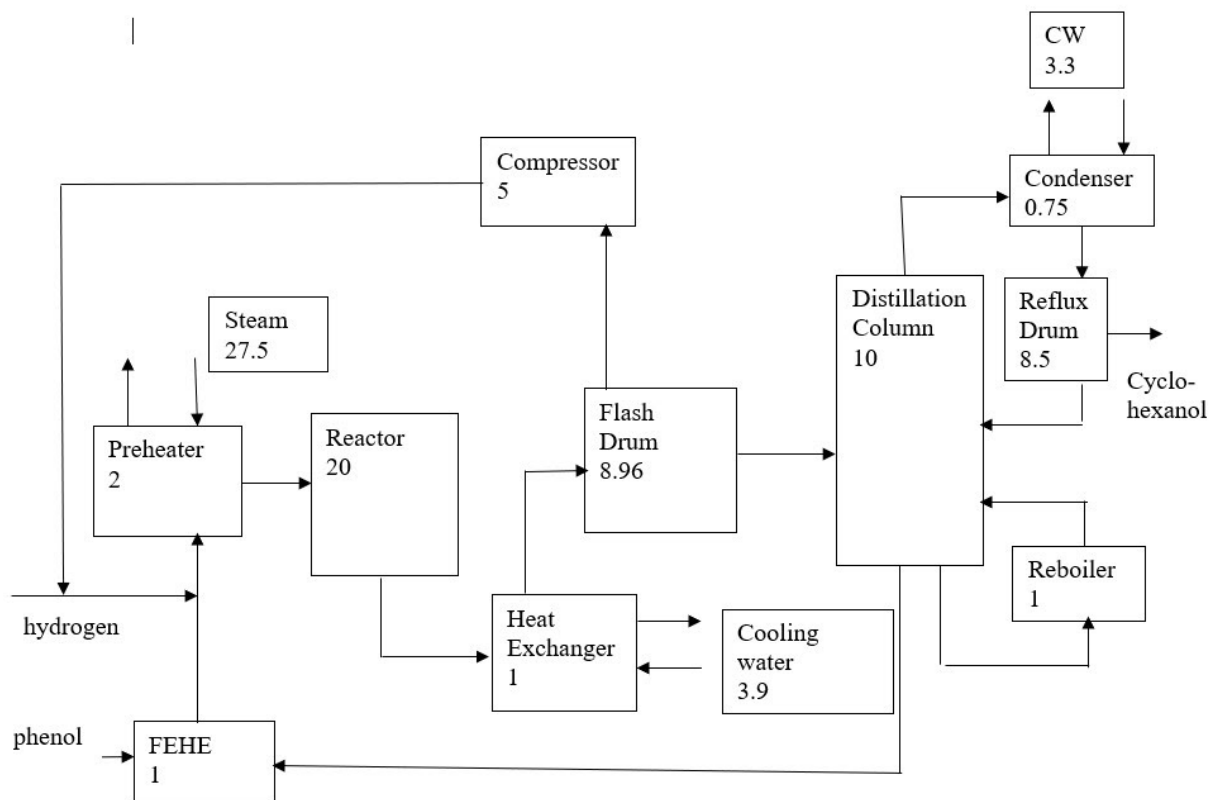
The reciprocal of the turnover ratio is sometimes defined as the capital ratio or the investment ratio.

Turnover ratio of 5 = Common for some business establishments.

Turnover ratio of 1 = Chemical industry.

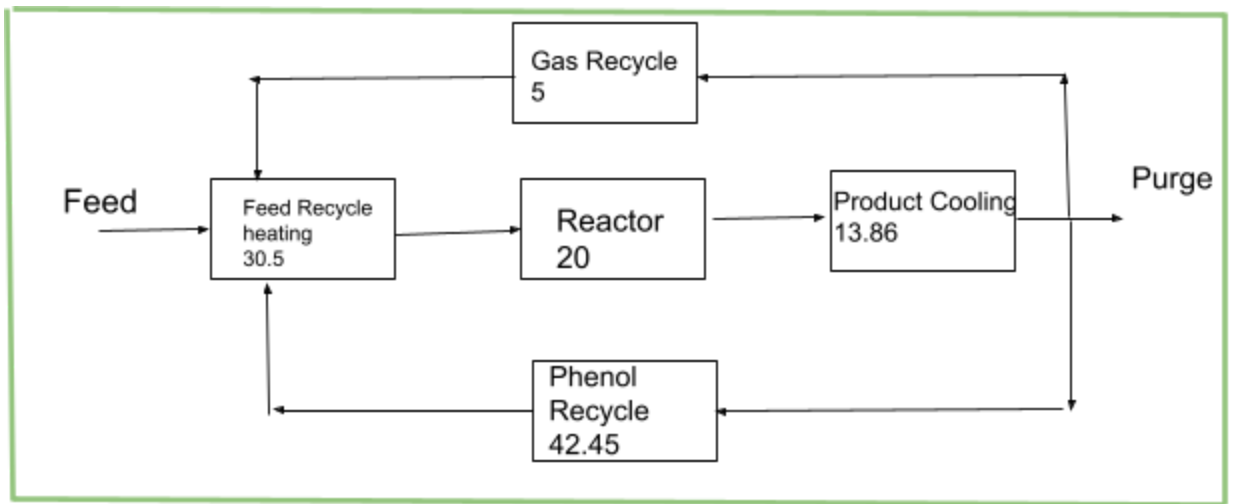
COST DIAGRAM FOR COMPLEX PROCESS

Cost in Rs. $x * 100000$.



Lumping

For the purpose of evaluating process alternatives, there is no advantage to treating the annualized capital cost and the annual power cost of the compressor separately. Hence, we combine these values into a total annual compression cost. Similarly, we should lump the capital and operating costs for both the furnace and partial condenser, and we combine the column, reboiler, condenser, steam, and cooling-water costs for the distillation column into a single separator cost value.



ESTIMATION OF REVENUE

Annual Sales Revenue = $\Sigma(\text{sales of product})(\text{product sales price})$

- Estimation of total product cost :

Total product cost = Manufacturing costs + General Expenses

(Here total product cost is calculated on an annual basis.)

□ Manufacturing costs:

Manufacturing costs = Variable production costs + Fixed charges + Plant-overhead costs

➤ Variable production costs-

Variable production costs include expenses directly associated with the manufacturing operation

1. Raw material cost = 107.40785 lakh/year

2. Utilities cost = 7.52 lakh/year
3. Operating labor costs = 20.15 lakh/year
4. Maintenance costs = 20.46 lakh/year

➤ Fixed Charges:

Fixed charges are expenses which remain practically constant from year to year and do not vary widely with changes in production rate.

1. Depreciation = 27.28 lakh/year
 2. Property taxes, Insurance = 10.23 lakh/year
- Plant-overhead cost = 13.7 lakh/year

□ General Expenses: 19.5 lakh/year + 13.58 lakh/year = 33.08 lakh/year

Total Product cost = 239.83 lakh = 2.4 lakh/ton

Revenue = 430 lakh/year (429.76 lakh/year)

★ Profit:

Profit before taxes-

1. Gross profit = Revenue - Total product cost = 430 - 239.83 = 190.17 lakh/year
2. After depreciation = 190.17 - 27.28 = 162.89 lakh/year
3. Profit after taxes = 162.89 - 10.23 = 152.66 lakh/year

❖ Stream factor :

No plant is capable of running all the time, since mechanical breakdown, maintenance, power disruption, shortage of feed or sale, cleaning or catalytic change, and so forth, cause it to periodically shut down. The fraction of time that the plant is operating in a calendar year is known as the on-stream factor

or stream factor (SF). No plant is capable of running all the time, since mechanical breakdown, maintenance, power disruption, shortage of feed or sale, cleaning or catalytic change, and so forth, cause it to periodically shut down. The fraction of time that the plant is operating in a calendar year is known as the on-stream factor or stream factor (SF).

$$\text{Stream Factor SF} = \text{Number of days plant operational per year} / 365 = 340 / 365 = 0.93$$

❖ Cost of capital:

No interest costs are included. This assumes that all the necessary capital comes from internal corporate funds, and comparisons to alternative investments must be on the same basis.

❖ Profitability analysis:

Profitability Standards:

- A profitability standard is a quantitative measure of profit with respect to the investment required to generate that profit.
 - a. Two standards:
 - Based on cost of capital (amount paid for the use of capital from sources such as bonds, common and preferred stock, and loans) Argument: Any project must earn at least the rate just to repay these external capital sources.
 - Minimum acceptable rate of return

Minimum Acceptable Rate of Return(MAAR):

- ❑ A commonly used profitability standard is the minimum acceptable rate of return (MARR).

MARR (M_{ar}): Rate of earning that must be achieved by an investment in order for it to be acceptable to the investor (expressed as a percentage per year). The highest rate of earning on alternate safe investments that is available to the investor - most commonly used basis

Here, minimum MAAR = 4% / year. (safe investment opportunities)

■ Methods to Calculate Profitability:

Methods That Do Not Consider the Time Value of Money:

1. Return on Investment (ROI) 2. Payback Period

➤ Return on Investment = $N_p / T = 152.66 / 344 = 44\%$.

$ROI \geq \text{minimum MARR}$

Therefore, The company is acceptable for the investor.

➤ Payback perio: Payback period (PBP), is the length of time necessary for the total return to equal the capital investment.

- Manufacturing fixed-capital investment = $V = 206.74$
- Non-manufacturing fixed-capital investment = $A_x = 33.08$
- Annual cash flow = $A_j = 152.66$

Payback period = $(V + Ax) \div Aj = 1.57 \text{ yr}$

Result and Conclusions

In this project, to get the final flowsheet we proceed through the hierarchy of decisions. We have done a literature survey to get max knowledge and ideas related to our project. Firstly we choose a process type which is a continuous process because we are asked to produce 100 tons/day.

After we have done material balance for input-output in the process and then decided the recycle structure of the process which is the very important part of the process, we use two recycle streams, one for hydrogen gas and the other for phenol. After that we did a separator structure analysis from which we decided to select a distillation column. Since we have both liquid and vapor phase components in the product and recycle streams. After that, we went for the energy balance in which we did separate energy balance for the mixing of Phenol and Hydrogen, for the Reactor and then for the distillation column. We have to supply more energy for the reactor than the mixing and separation process. Then we came up with the final flow sheet by which we can produce Cyclohexanol in an effective and profitable manner. Then we went for the design of a heat exchanger which is very essential for controlling heat energy. For establishing the plant we went for the selection of proper equipment. We have chosen a PFR reactor, a distillation column, a Reflux drum, a Reboiler, a Condenser, a Compressor, a Evaporator, Flash Drum, Pumps, Valves and Pipes in which we have to invest approx 70 lac. We estimated our total cost and calculated total capital investment in establishing the plant. We calculated the direct cost which includes Equipment purchasing, Equipment Installation, Piping (includes insulation), Instruments & Control , Electrical Equipment, Buildings(Process,Administration, Maintenance shops etc),

Site Preparation, Service Facilities (steam, air, water, fuel, electricity etc.), Land and indirect cost which includes Engineering & Supervision (Administrative and design, Supervision and Inspection), Construction Expenses, Contractor's fee, Contingency and Start-up expenses. We estimated capital investment by different methods. We took the prices of equipment and material from the internet. Then we calculated the percentage of delivered equipment cost. Then we drew the cost diagram for the complex process. We calculated the total product cost which is 239.83 lakh/year, General expenses which is 33.08 lakh/year and Revenue which is 430 lakh/year. After that we calculated gross profit to be 190.17 lakh/year and profit after depreciation and taxes to be 152.66 lakh/year. At the last we performed profitability analysis. Based on ROI method we found that our process gains profit and is suitable for the investors to invest. The minimum payback period to get the capital investment is 1.57 year.

References

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