An Efficient Design of Multi Component Distillation Column by Approximate & Rigorous Method

Syed Mujahed Ali Rizwan
Senior Lecturer in Chemistry
Challenger College,
Moinabad, Hyderabad.

Abstract:

In this paper we have described methodology to separate three components (hexane, heptanes and octane) by approximate and rigorous method. Approximate method includes three steps for the calculation of minimum stages; minimum reflux ratio and calculation of actual number stages for the distillation column. We have started with choosing key and non-key components. Then we have calculated temperature of re-boiler and condenser by bubble point and dew point calculation. After that we have calculated minimum number of stages by using Fenske equation, minimum reflux ratio with the help of under wood equation. We have taken actual reflux ratio as 1.5 times of minimum reflux and then we have calculated theoretical stages by using Gilliland equation at which distillation column will operate. After that we have performed rigorous calculations by Lewis Matheson method to obtain temperature and compositions of all the three components at each tray.

INTRODUCTION

Separation process principles

The creation of a mixture of chemical species from the separate species is a spontaneous process that requires no energy input. The inverse process, separation of a chemical mixture into pure components, is not a spontaneous process and thus requires energy. A mixture to be separated may be single or multiphase. If it is multiphase, it is usually advantageous to first separate the phases. A general separation schematic is shown in Figure 1.1 as a box wherein species and phase separation occur, with arrows to designate feed and product movement.
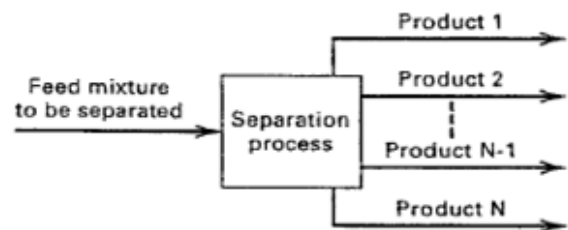

Figure 1.1: General separation process

The feed and products may be vapor, liquid, or solid; one or more separation operations may be taking place; and the products differ in composition and may differ in phase. In each separation operation, the mixture components are induced to move into different, separable spatial locations or phases by any one or more of the five basic separation methods shown in Figure1.2. However, in most instances, the separation is not perfect, and if the feed contains more than two species, two or more separation operations may be required. The most common separation technique, shown in Figure1.2a, creates a second phase, immiscible with the feed phase, by energy (heat and/or shaft-work) transfer or by pressure reduction. Common operations of this type are distillation, which involves the transfer of species between vapor and liquid phases, exploiting differences in volatility (e.g., vapor pressure or boiling point) among the species; and crystallization, which exploits differences in melting point. A second technique, shown in Figure 1.2b, adds another fluid phase, which selectively absorbs, extracts, or strips certain species from the feed. The most common operations of this type are liquid–liquid extraction, where the feed is liquid and a second, immiscible liquid phase is added; and

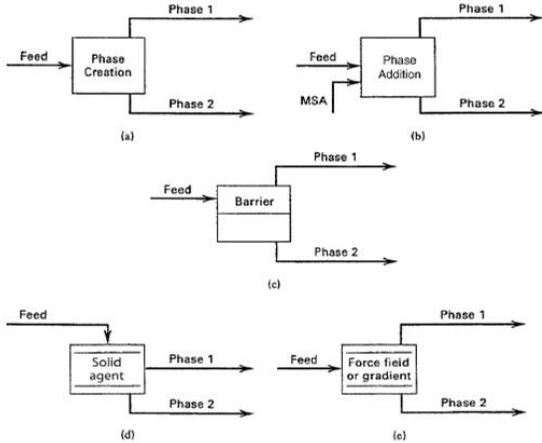absorption, where the feed is vapor, and a liquid of low volatility is added.

Figure 1.2: Basic separation technique; (a) separation by phase creation; (b) separation by phase addition; (c) separation by barrier; (d) separation by solid agent; (e) separation by force field or gradient

In both cases, species solubility's are significantly different in the added phase. Less common, but of growing importance, is the use of a barrier (shown in Figure 1.2c), usually a polymer membrane, which involves a gas or liquid feed and exploits differences in species permeability's through the barrier. Also of growing importance are techniques that involve contacting a vapor or liquid feed with a solid agent, as shown in Figure 1.2d. Most commonly, the agent consists of particles that are porous to achieve a high surface area, and differences in species adsorb ability are exploited. Finally, external fields (centrifugal, thermal, electrical, flow, etc.), shown in Figure 1.2e, are applied in specialized cases to liquid or gas feeds, with electrophoresis being especially useful for separating proteins by exploiting differences in electric charge and diffusivity. For the techniques of Figure 1.6, the size of the equipment is determined by rates of mass transfer of each species from one phase or location to another, relative to mass transfer offal species. The driving force and direction of mass transfer is governed by the departure from thermodynamic equilibrium, which involves volatilities, solubility's, etc.

Distillation

In distillation (fractionation), a feed mixture of two or more components is separated into two or more products, including, and often limited to, an overhead distillate and bottoms product, whose compositions differ from that of the feed. Most often, the feed is a liquid or a vapour–liquid mixture. The bottoms product is almost always a liquid, but the distillate may be a liquid, a vapor, or both. The separation requires that: (1) a second phase be formed so that both liquid and vapor are present and can make contact while flowing counter currently to each other in a traded or packed column, (2) components have different volatilities so that they partition between phases to different extents, and (3) the two phases are separable by gravity or mechanical means. Equipment for continuous distillation is shown in fig. (1.3)
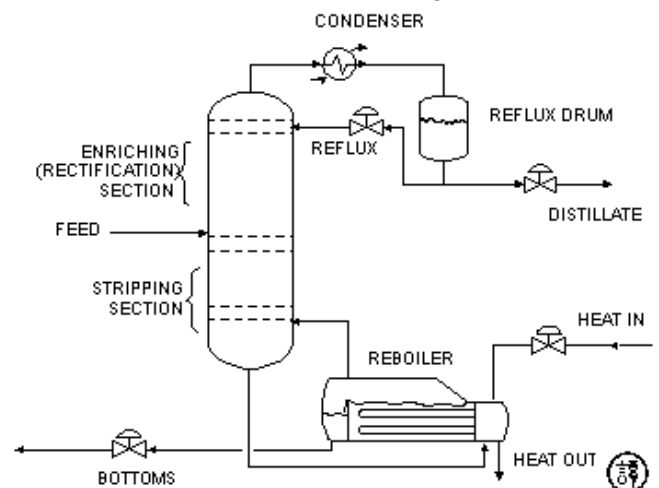

Figure 1.3: A continuous distillation column

Distillation column is fed continuously with liquid mixture to be distilled and the liquid in the reboiler is partially converted to vapour by heat transferred from the heating element inside the reboiler. The vapour stream rising from the reboiler is brought in to intimate counter current contact with a descending stream of liquid in the column. This liquid must be rich enough in the low boiler that there is mass transfer of the low boiler from the liquid to the vapour at each stage of the column. Such a liquid can be obtained simply by condensing the overhead vapours and returning some of the liquid to the top of the column. This return

liquid is called reflux. The reflux entering the top of the column is often at the boiling point but if it is cold, it is almost immediately heated to its boiling point by the vapour. Throughout the rest of the column, the vapour at any stage is at the same temperature as the liquid, which is at its boiling point. The temperature increases on going down the column because of the increase in pressure and the increasing concentration of high boiling components. The plate on which the feed enters is called feed plate. All plates above the feed plate constitute the rectifying section and all the plates below the feed, including the feed plate itself, constitute the stripping section. The vapours rising through the rectifying section are completely condensed in a condenser and the condensate is collected in accumulator, in which a definite liquid level is maintained.The separation of components that have nearly the same boiling points is difficult by simple distillation even if the mixtures are ideal, and complete separation may be impossible because of azeotropes formation. For such systems the separation can often be improved by adding a third component to alter the relative volatility of the original components. The added components may be a higher boiling liquid or solvent that is miscible with both of the key components. The key components that are more like the solvent will have a lower activity coefficient in the solution then the other component, so the separation is enhanced. This process is called 'Extractive Distillation' and is like liquid- liquid extraction with an added vapour phase.

Raoult's law:

Raoult's law is a law of thermodynamic established by French physicist Francois-Marie Raoult in 1882. It states that the partial vapour pressure of each component of an ideal mixture of liquids is equal to the vapour pressure of the pure component multiplied by its mole fraction in the mixture.

Thus the total pressure above solution of A and B would be:

$$P_T = P^{\circ}_A x_A + P^{\circ}_B x_B \quad eq (1.5.1)$$

Where, P_T = total pressure

P°_A, P°_B = saturation pressure of component A and B respectively

x_A, x_B = mole fraction of component A and B respectively

Dalton's law:

Dalton's law states that the total pressure exerted by the mixture of non-reactive gases is equal to the sum of the partial pressures of individual gases. This empirical law was observed by John Dalton in 1801 and is related to the ideal gas laws.

Mathematically, the pressure of a mixture of gases can be defined as the summation:

$$P_{total} = \ldots eq (1.5.2)$$

Where,   pi = partial pressure of each component

THEORY

In multicomponent distillation, as in the distillation of binary mixtures, the calculation of equilibrium stages uses mass and enthalpy balances and vapours liquid equilibria. A mass balance can be written for each component for the column as a whole or for a single stage, but there is only one enthalpy balance for the column or for each stage. The phase equilibria are much more complex than for binary system, because of the several components and because the equilibria depends on temperature, which changes from stage to stage.In binary system the temperature and equilibria also change from stage to stage except with azeotropes. The more volatile component is alwaysmore volatile than the other component throughout the column. In multicomponent mixtures one component may be more volatile than the average in one part of the column and less volatile than the average in another part, which leads to complex concentration profiles. In practice the field is dominated by the use of computers because of the mass of numbers needed to quantify the operating and engineering variables and the many iterations required to obtain convergence of the solution to the equations.

Although rigorous methods are available for solving multicomponent separation problems, approximate methods continue to be used for preliminary design, parametric studies to establish optimal design conditions, process synthesis studies to determine optimal separation sequences, and to obtain initial approximations for rigorous, iterative methods.

Table 1: Properties of Paraffin

S.No.	Component	molecular formula	Density (gm /ml)	Boiling point (deg. C)	Melting point (deg. C)
1.	Hexane	C_6H_{14}	0.6548	69	-96
2.	Heptane	C_7H_{16}	0.6795	99	-93
3.	Octane	C_8H_{18}	0.7030	125	-57

Approximate method

An approximate method for preliminary design and optimization of simple distillation is the Fenske–Underwood–Gilliland (FUG) method.Fig. 2.1gives an algorithm for the FUG method, namedafter the authors of the three steps in the procedure, whichwill be applied to the distillation column. These methods are sampled as: the estimate of the minimum number of plates, minimum reflux ratio and calculation of ideal number of stages.
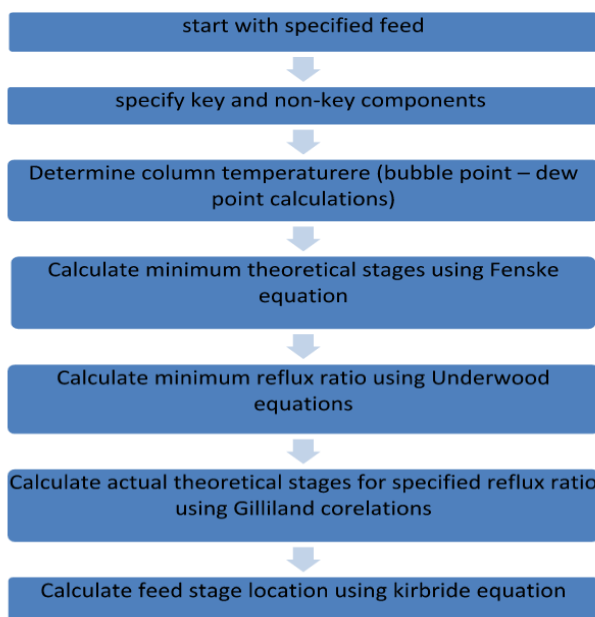

Figure 2.1: algorithm for multicomponent distillation column using FUG method

PROCEDURE

This is procedure for a sample mixture of 50% n-hexane, 40% n-heptane and 10% n-octane. Total column operating pressure is taken as 1 atm. Distillate and reboiler compositions are calculated on the basis of 98% recovery of hexane and 1% of heptane in the distillate by simple material balance equations.

Calculation of mole fractions of distillate and bottom product

Distillate calculations
Moles of hexane: F*xfhex*0.98 =100*0.5*0.98= 49
Moles of heptane:F*xfhept*0.01=100*0.4*0.01=0.4
Mole of octane = 0 (since, it is heavier than heavy key)
Total moles =49+0.4+0 = 49.4
Mole fraction of hexane = 49/49.4 = 0.9919
Mol fraction of heptane = 0.4/49.4 =0.008
Mole fraction of octane = 0/49.4 = 0
Bottom calculations
Moles of hexane: Fxfhex*0.02=100*0. 5*0.02=1
Mole of heptane: F*xfhept*0.99= 100*0.4*0.99= 39.6
Moles of octane: F*xfbottom*1=100*0.1*1=10
Total moles = 1+39.6+10= 50.6
Mole fraction of hexane = 1/50.6= 0.0197
Mole fraction of heptane = 39.6/50.6 = 0.7826
Mole fraction of octane = 10/50.6 = 0.1976

Selection of key and non key components

In multicomponent distillation, there are three or more components in the product and specifying the concentration of one component in each does not fully characterise these products. So we have to choose two components whose concentration in the distillate and bottom products are a good indication of separation achieved. Now it is assumed that most of the light components lighter than light key ends up in the distillate and the heavy components heavier than heavy key ends in the bottom products. Although any two components can be nominated as keys, they are adjacent in the rank order of volatility. Such a choice is called sharp separation. In sharp separation the keys are the only components that appear in both products in appreciable concentration.We have selected hexane

as light key component and heptane as heavy key component.

Bubble point calculationsfor condenser and reboiler

For bubble point calculation, the liquid composition is known and the total pressure is given. We start with an assumed temperature and calculate the vapour pressure or K-values of all the components then we calculate the value of Kixi (Ki =P^o/PT). Saturation pressure is calculated by usingAntonie equation at assumed temperature.

At bubble point:∑Kixi=1

If the summation ≠ 1, than choose another temperature and continue the iterations until the summation does not approaches 1.

For a temperature of 341.8°C following data is obtained

Table 2: Bubble point calculation

S.No.	Components	Partial Pressure (atm)	K_i	X_i	K_iX_i
1.	Hexane	0.9869	0.9953	0.9919	0.9872
2.	Heptane	0.3797	0.3798	0.0081	0.00307
3.	Octane	0.1480	0.1480	0.0	0.0
	Total				0.9903

RESULT

Temperature of Condenser	:	341.7000
Temperature of Reboiler	:	378.8000
The value of Relative Volatility	:	2.6209
Minimum number of trays required:		7.8084
Minimum Reflux Ratio	:	1.0564
Actual Reflux Ratio	:	1.5846
Required number of stages	:	17
Stages in stripping section	:	10
Stages in rectifying section	:	7
Feed plate location	:	10

Table 4: temperature and liquid composition on the trays

Tray no. (starting from bottom tray)	Temperature (°K)	Liquid Composition		
		hexane	heptane	octane
1	373.9	0.0285	0.9061	0.1095
2	372	0.0520	0.9062	0.0858
3	370.6	0.0882	0.8801	0.0771
4	368.9	0.1406	0.8312	0.0731
5	366.7	0.2093	0.7644	0.0705
6	364.1	0.2893	0.6876	0.0682
7	361.2	0.3678	0.6099	0.0661
8	358.6	0.4347	0.5449	0.0643
9	356.6	0.4850	0.4975	0.0631
10	352.3	0.5457	0.4316	0.0228
11	349.8	0.6345	0.3576	0.0078
12	347.5	0.7268	0.2708	0.0025
13	345.5	0.8119	0.1873	0.0007
14	344	0.8811	0.1187	0.0002
15	343	0.9312	0.0687	0.0000
16	342.3	0.9646	0.0354	0.0000

CONCLUSION AND SUMMARY

Generally, chemical process industries involve distillation of a mixture of several components rather than that of a binary mixture. Designing by approximate and rigorous method gives an initial analysis of a multicomponent distillation column design. To start designing with these methods, distillate and bottom recoveries must be predecided. Approximatemethod gives minimum number o f stages, minimum reflux ratio, actual reflux ratio and ideal number of stages. Rigorous method gives temperature and concentration of component on each tray.

The results obtained from these methods are than analysed to determine the correct specifications for the operations of a real distillation column. This is done by experience from past or from literature work.

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