Engineering design of second distillation column of IPA

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Abstract. This research work is about design of second distillation column in a continuous flow process for isopropylalcohol (88% purity) producing (Cumene process) for industry. The differences between tray and packed column were observed and the preference was given to the one with most advantageous abilities. Some technical (engineering) calculations were solved within this project to choose accurate properties for the distillation column.

1. Introduction

Distillation is plays the separation role of liquid mixtures into some components or fractions by selecting the boiling point (evaporation) of each component and the condensation [1]. In distillation process, there should be at least one feed going in and at least two outputs (top and bottom operating flows). In this project on second distillation column the separation of isopropylalcohol (IPA) from water should be preceded, where IPA contains 22% of water and small amount of acetone (acetone has been calculated as a very small amount, so it’s negligible) and will be fed back to T-junction (mixing point). Consequently, IPA in water mixture has been considered as a binary system [2]. The feed enters to the distillation operates at a pressure of 1 atmosphere absolute pressure.

There are lots of types of the distillation columns and each of them is designed differently from each other in terms of complexity, where the main idea is to perform specific type of separation procedure. As the process is continuous, the choice of distillation column will be between tray and packed column. Choose of the distillation column for a given mass transfer operation should be based “theoretically” on detailed cost studies for the two types of contractors. However, the primacy can be made on the basis of qualitative consideration of relative advantages and disadvantages, excluding the need for a detailed cost comparison [3].

An advantage of having packed column is that has a lower pressure drop across the column and even more beneficial when the operation is under vacuum. If the distillation tower will be using packing, the needed theoretical equilibrium stages can be determined and then the packing height can be determined comparable to a theoretical equilibrium stage as well. The number of the theoretical stages needed to proceed for a given separation can be calculated by using a specific vapour to liquid ratio. If liquid and vapour are not distributed across the superficial area as it enters the packed bed, the ratio between vapour and liquid will be wrong in the packed bed and the separation will not proceed so, the packing will occur to work not properly. The packing material can be structured sheet metal or Rasching rings. The problem with this issue is not the packing itself, however the mal -distribution of
the feed entering the packed bed. The design of the liquid mal – distributors is used to introduce the feed and reflux to packed bed.

The idea of a tray is to provide intimate mixing between the vapour steam and liquid, so it should be suitable for receiving the desired rates of liquid and vapour with excessive flooding. A tray should be stable in operation and it should be quite easy to erect and maintain.

Distillation can be classified as:
Counter – current trays without down – comers (figure 1)
Cross – flow trays with down – comers (figure 2)

The counter – current trays allows liquid and gas to pass through the same tray opening, which results in a limited operating range due to the sensitivity of dispersion height to the liquid / gas flow rates. In other words, counter – current trays are used only in cases where, high resistance or high capacity to the fouling and because of its small operating range, the market is small as well, so such a type of trays are not suitable in this case. The purpose of down – comers is to provide a conduit for the frothy liquid to flow to the tray desk below. Any significant amount of liquid / vapour traveling out the bottom of the down – comers should be avoided, because it will reduce the tray efficiency and capacity due to back - mixing.

**Figure 1.** Counter – current trays without down – comers.

**Figure 2.** Cross – flow trays with down-comers.

The arrangements for the liquid flow over the tray depends on the ratio of liquid to vapour flow, so there are different layouts (figure 3)

**Figure 3.** Arrangements for liquid flow over the tray.
Cross flow – gives good opportunity for mass transfer and it is good with length of liquid period.
Reverse flow – in this type of flow, the down-comers are reduced very well, suitable for low liquid vapour ratios
Double – pass flow – in this case, the liquid flow is splits into two directions, so this flow will be good for high liquid vapour ratios.
As in this project very much amount of liquid needs to be processed, so the cross flow are used.

2. Results and discussion
The feed entering the column is a mixture of 59.80 kg moles of IPA, 0.79 kg moles of acetone and 1418.24 kg moles of water (steam 22). The feed inlet temperature is 23.50°C where the distillate product (78% IPA and 22% of water) temperature is 250°C at 1.1 bar at steam number 23 and the bottom product (assumed as pure water but with small amount of IPA, which is negligible) at 1000°C at 0.96 bar at steam number 29.

**Ipa/water distillation column**

\[ V = \text{vapour – liquid leaving} \]
\[ q = \text{Feed quality (L/L)} \]
\[ L = \text{vapour - liquid coming} \]
\[ V_2 \text{ vapour liquid coming} \]
\[ L_2 \text{ vapour liquid leaving} \]

![Distillation Unit 2](image)

**Figure 4.** Illustration diagram for the IPA/water distillation column.

Assumptions: Assumptions are made according to Couslon and Richardson’s suggest, page 589-590
Plate spacing – 5 mm
Pressure drop per plate – 100 mm
Flooding – 85%
Weir Height – 50 mm
Plate thickness – 5 mm
Hole diameter = 3 mm
The feed component:

|          | inlet kmols | distillate outlet kmols | bottoms outlet kmols |
|----------|-------------|-------------------------|----------------------|
| IPA      | 7.9000      | 7.80                    | 0.1000               |
|          | 473.9100    | 467.834                 | 6.076                |
With the relative volatility value (alpha) = 2.23 (J.D. Seader, E.J. Henkey, D.K. Roper. Separation Process Principles (3-rd Ed.) J. Wiley & Sons Inc., New York, 2011) the following data table (Table 2) of values were calculated with $y_1 = \frac{\alpha x_1}{1+x_1(\alpha-1)}$ Eq. 1 and the data were used for the vapour liquid equilibrium curve:

**Table 2. Equilibrium data for IPA/water mixture.**

|   |     |     |     |     |     |     |
|---|-----|-----|-----|-----|-----|-----|
| Water | 624.39 | 11239.07 | 2.23 | 40.140 | 622.16 | 11198.93 |
| Acetone | 0.1100 | 6.260000 | 0.00 | 0.0000 | 0.1100 | 6.260000 |
| TOTAL | 632.40 | 11719.24 | 10.03 | 592.39 | 622.17 | 11205.19 |

An example of worked calculation: shown at $x = 0.5$

$by \ using \ Eq. 1 \ y_5 = \frac{2.23 \times 0.5}{1 + 0.5 \times (2.23 - 1)} \Rightarrow \ y_5 = 0.6043$

The following graph equilibrium graph (figure 5) was plotted by using the calculated values of $x$ and $y$.

![Equilibrium graph of IPA/Water mixture (azeotrope).](image-url)
From the figure above (figure 6) it the highest purity of distillate IPA can be determined to be only at 80% of IPA (in ideal), where the rest is water, but it was estimated that the distillate product will be $x_D = 78\%$ of IPA and $x_W = 22\%$ of water.

Calculations for the number of plates with using Fenske Method (eq. 11.58 Coulson & Richardson Chemical Eng. Vol 2, 5-th Ed)

$$N_{\min} + 1 = \frac{\ln\left(\frac{X_D}{X_W}\right)d\left(\frac{X_D}{X_W}\right)}{\ln(\alpha)} \quad Eq. \, 2 \Rightarrow N_{\min} + 1 = \frac{\ln\left(\frac{0.78}{0.22}\right)\left(\frac{0.98}{0.02}\right)}{\ln 2.23} \Rightarrow N_{\min} = 6.43 \text{ or 7 stages (rounded)}$$

Calculating $R_{\text{MIN}}$ with using an Underwood’s Equation (Eq. 11.114 Coulson & Richardson Chemical Eng. Vol. 2, 5-th Ed).

$$R_{\text{MIN}} + 1 = \sum \frac{\alpha^D}{\alpha - \theta} \Rightarrow R_{\text{MIN}} + 1 = 4.38$$

Minimum reflux ratio $R_{\text{MIN}} = 3.38$

With Gilland correlation for calculating number of stage:

$R = 1.28$ (for IPA/water) (J.D. Seader, E.J. Henkey, D.K. Roper. Separation Process Principles (3-rd Ed.) J. Wiley & Sons Inc.,New York, 2011)

$R=1.28 \times R_{\text{MIN}} \Rightarrow$

$R = 4.33$, Therefore,

$$\frac{R - R_{\text{MIN}}}{R + 1} \Rightarrow \frac{4.33 - 3.38}{4.33} = 0.18$$

From Gilland Correlation (Figure 1.6) the $\frac{N - N_{\min}}{N + 1}$ can be calculated

![Figure 6. Gilland Correlation table.](image)

So, from the above table (Figure 1.6) \(\frac{N - N_{\min}}{N + 1} = 0.47\)

$$\frac{N}{N + 1} = 13 \text{ stages}$$

Assumptions:
Pressure drop per plate – 100mm
Isopropyl alcohol – 710 Pa
Column pressure drop = 710*RMM \( \rightarrow \) 710*60.10=42671Pa
Pressure_{bottom} = 1\text{ bar} + 42671 \text{ Pa} = 101325 + 42671 = 143996\text{ Pa}

The temperature at bottom operating sections is 100°C

Top operating section the temperature is 25°C

So, the density of top product at 25°C will be \( p_l = 768 \text{ kg/m}^3 \) (\( p_v = 1.3 \text{ kg/m}^3 \))

The density of bottom product= \( p_l = 958.4 \text{ kg/m}^3 \) (\( p_v = 1.67 \text{ kg/m}^3 \))

Molecular weight will be same at top and bottom operating section = \( MW_{IPA} + MW_{water} = 60.1+18.02 = 78.12 \)

Acetone is also presented, but very less amount, so it’s negligible and kept as 0.

For top product:
\[
\begin{align*}
L_n &= R*D = 4.33*7.8 = 33.77 \\
V_n &= R+D= 33.77+67.96 = 101.73
\end{align*}
\]

For bottom product:
\[
\begin{align*}
L_m &= L_n + F = 33.77 + 632.4= 666.17 \\
V_m &= L_m - W = 101.73
\end{align*}
\]

To minimise an entrainment the tray spacing is selecting. Vacuum columns are needed for a large distance between the trays. A trial spacing of 0.45 was selected.

The column diameter can be designed with using “Liquid – vapour flow factor \( F_{LV} \)” (figure 7) from Coulson & Richardson Chem Eng Vol. 6, 4-th Ed

\[
\begin{align*}
F_{LV} &= \frac{L_w}{V_w} \times \sqrt{\frac{p_v}{p_L}} \quad \text{Eq. 3}
\end{align*}
\]

Where \( L_w \) = liquid mass flow rate kg/s
\( V_w \) = vapour mass flow rate kg/s

Consequently,
\[
\begin{align*}
F_{LV \_top} &= 0.03 \\
F_{LV \_bottom} &= 0.05
\end{align*}
\]

Bottom and top \( K_1 = 0.08 \)

From Liquid – Vapour correlation factor \( K_1 \) can be determined as 0.147 at 0.45mm spacing

3. Flooding velocity
From Coulson & Richardson Chem. Eng. Vol. 6, 4-th Ed
Where $U_f = \text{flooding vapour velocity, m/s}$

$K_1 = \text{a constant that obtained from Vapour - Liquid correlation graph, so by using Eq. 7 for top and bottom operating process}$

\[
\mu_{f_{\text{top}}} = 0.08 \times \sqrt{\frac{768 - 1.3}{1.3}} = 1.94 \text{ m/s}
\]

\[
\mu_{f_{\text{bottom}}} = 0.08 \times \sqrt{\frac{958.4 - 1.67}{1.67}} = 1.91 \text{ m/s}
\]

Design for 85% flooding at maximum flow rate

\[
\mu_{v_{\text{top}}} = 0.85 \times 1.94 = 1.66 \text{ m/s}
\]

\[
\mu_{v_{\text{bottom}}} = 0.85 \times 1.91 = 1.63 \text{ m/s}
\]

Maximum volumetric flow rate

\[
\text{Bottom} = \frac{V_n \times MW}{p_v \times 3600} = \frac{101.73 \times 78.12}{1.67 \times 3600} = 1.322 \text{ m}^3/\text{s}
\]

\[
\text{Top} = \frac{V_m \times MW}{p_v \times 3600} = \frac{101.73 \times 78.12}{1.3 \times 3600} = 1.700 \text{ m}^3/\text{s}
\]

Net area required

\[
A_{n_{\text{TOP}}} = \frac{Q_v}{Q_n} = \frac{1.700}{1.66} = 1.020 \text{ m}^2
\]

\[
A_{n_{\text{BOTTOM}}} = \frac{Q_v}{Q_n} = \frac{1.322}{1.63} = 0.811 \text{ m}^2
\]

Down-comer area is suggested as 12% in Coulson & Richardson’s Chem. Eng. Vol. 6, 4-th Ed.

Column cross-sectional area

\[
top = \frac{1.700}{0.78} = 2.180 \text{ m}^2
\]

\[
bottom = \frac{0.811}{0.78} = 1.040 \text{ m}^2
\]

Down-comer Area

\[
\text{Top} = \frac{12 \times 2.18}{100} = 0.262 \text{ m}^2
\]

\[
\text{Bottom} = \frac{12 \times 1.040}{100} = 0.125 \text{ m}^2
\]

Column Diameter

\[
\text{Top} = \frac{4}{\pi} \times \sqrt{2.18} = 1.88 \text{ m}
\]

\[
\text{Bottom} = \frac{4}{\pi} \times \sqrt{1.040} = 1.300 \text{ m}
\]

So the column diameter is 1.88m
4. Conclusion

To sum up the vapour liquid equilibrium curve was plotted with \( x_D = 78\% \) of IPA and \( x_W = 22\% \) of water and the number of plates by using Fenske Method also were calculated to 7 (rounded). The minimum reflux ratio \( R_{MIN} \) was calculated as 3.38, therefore, by using the Gilland Correlation table, the number of stages were calculated to be 13. Tray spacing was calculated by using liquid – vapour flow factor \( K_1 \) as 0.147 at 0.45mm spacing. Net area at the top and bottom was calculated as 1.020 \( m^2 \) and 0.811 \( m^2 \) respectively. Flooding velocity at the top and bottom 1.94 m/s and 1.91 m/s correspondingly. The column diameter was calculated as 1.88m.

References

[1] Luyben W L 2011 Design and control of the acetone process via dehydrogenation of 2-propanol *Industrial and engineering chemistry research* **50** (3) 1206-18
[2] Majiburohman M, Sediawan W B and Sulistyo H 2019 A preliminary study: distillation of isopropanol-water mixture using fixed adsorptive distillation method
[3] Thong D Y-C and Jobson M 2001 Multicomponent homogeneous azeotropic distillation 2 column design *Chemical Engineering Design* **56**(14) 4393-416
[4] Patwardhan A A 1992 *Modelling and control of a packed distillation column* (Texas: The University of Texas at Austin)
[5] Samoilov N A and Mnushkin I A 2012 Mathematical modelling fractionation stage of reactive distillation process for production of ethylene glycol *Ufa State Petroleum Technical University* **4** 158-64
[6] Bamatov I 2017 Development Of The Chemical Reactor V-Star For Continuous Flow Reactions *Chechen State University Journal* **2** (6) 205-7