A comprehensive study was performed to optimize the separation of acetone and water by use of a valve tray distillation column. This report contains information regarding the design, specifications, sizing and the costing of the distillation column.

Prepared by: John Paul Handrigan
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Introduction

The separation of acetone and water in the cumene process is an important step in making the process economically viable since acetone is a valuable co-product. Often the decision the decision to produce phenol is dependent on the marketability of acetone.

In this particular distillation tower, T-402, the light key component is acetone as it is the product that is to be limited from the bottom product. The heavy key component is water, and it is desired to keep this out of the top product to recover acetone at high purity. Figure 1 is a simplified representation of tower T-402, which will be developed in this report.

Figure 1: Basic Representation of Distillation Tower T-402

In the above distillation tower, the acetone continues to a storage tank, while the water is treated in a wastewater treatment facility. The ideal purity of the acetone in the distillate is
based on the standard market purity which is a weight percentage of 99.5. This corresponds to a volume percentage of 98.4.

Other common methods of acetone/water separation include extractive distillation. The extractive distillation can be performed with the addition of diethylene glycol dimethyl ether, or diglyme among others (Okullo, 1999). The extractive distillation method would achieve a higher purity of acetone in the distillate, but would require the addition of a second tower in order to separate the water and diglyme. The second separation tower would be necessary in order to recover diglyme, which is an expensive organic solvent. A second tower may lead to higher capital costs, and also higher operating costs, but a further study would need to be performed to compare distillation versus the ternary extractive distillation. Another reason for choosing distillation over extractive distillation is that only a purity of 99.5% is required, whereas the extractive distillation is often used to obtain higher purities around 99.9% (Okullo, 1999).

Also, distillation was the optimal means of separation for acetone/water because of the significant difference in their boiling points, as shown in Table 1. It should be noted that even though distillation is appropriate for acetone-water separation, the high purity of acetone required for recovery is difficult to achieve and requires careful design.

**Table 1: Summary of Properties for Acetone and Water**

<table>
<thead>
<tr>
<th>Component</th>
<th>Molecular Formula</th>
<th>Molecular Weight (g/mol)</th>
<th>Boiling Point (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Acetone</td>
<td>C₃H₆O</td>
<td>58.08</td>
<td>56.05</td>
</tr>
<tr>
<td>Water</td>
<td>H₂O</td>
<td>18.01</td>
<td>100.00</td>
</tr>
</tbody>
</table>
Chapter 3: Process/Equipment Design

The design of a distillation column requires extensive research, careful calculations, and an overall economic analysis. In this chapter, the distillation column for the separation of acetone and water will be designed. The important parameters involved in the design of a distillation column include column diameter, column height, types of tray, tray efficiency, flooding velocity, and materials of construction.

The first step of the process for designing a distillation column is to determine the minimum reflux ratio, and the number of trays required to obtain the desired separation. There are several methods available for determining these design parameters for distillation towers, including the FUG method and the McCabe-Thiele method. The FUG method is an analytical approach, whereas McCabe-Thiele uses a graphical approach. Both of these methods have their merits, and were both in the design of the acetone-water distillation tower.

The inlet feed conditions used in both of these methods are required and have been summarized in Table 2.

Table 2: Summary Data for Feed Stream

<table>
<thead>
<tr>
<th>Condition</th>
<th>Feed Stream</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (K)</td>
<td>330.15</td>
</tr>
<tr>
<td>Pressure (kPa)</td>
<td>101.325</td>
</tr>
<tr>
<td>Acetone (mol %)</td>
<td>76.2</td>
</tr>
<tr>
<td>Water (mol %)</td>
<td>23.6</td>
</tr>
<tr>
<td>Oxygen (mol %)</td>
<td>0.1</td>
</tr>
</tbody>
</table>

*The mol% does not add to 100% as there are other components in small amounts

It was assumed that the effect of oxygen on the distillation would be negligible, and for this reason tower T-402 was modeled as a binary distillation tower.

The Fenske-Underwood-Gilliland’s (FUG) method is an analytical method for determining the number of equilibrium stages for multicomponent distillation. In tower T-402, there exists a multicomponent distillation since there is acetone, water and very minute amounts of oxygen.
Since there is only a very minute amount of oxygen, the McCabe-Thiele method may also be valid for a binary distillation, which will be explored. Detailed design calculations pertaining to the FUG method and McCabe-Thiele method have been outlined in Appendix C.

First of all, the Fenske relation was used to determine the minimum number of stages. One of the assumptions made for this relation is that components lighter than the light key will exit in the distillate, and components heavier than the heavy key will exit in the bottoms. Using the Fenske relation it was determined that the minimum number of stages required for the separation of acetone-water is 5.1 stages. Detailed calculations to determine the minimum number of stages has been outlined in Appendix C.

![Figure 2: VLE Data for Acetone-Water at 101.325 kPa](image)

Figure 2: VLE Data for Acetone-Water at 101.325 kPa

Once the minimum number of stages has been determined, it is possible to use Underwood’s method to determine the minimum reflux in the distillation tower. For tower T-402 it was determined that the minimum reflux had a value of approximately 0.483. The minimum reflux
value found using Underwood’s method differed considerably from the value determined using the McCabe-Thiele method. The vapour-liquid equilibrium (VLE) data required for the McCabe-Thiele is shown in Figure 2 for an acetone-water mixture at atmospheric pressure. Using this graph, while plotting the stripping and enriching lines it was possible to determine the number of theoretical stages, and also a minimum reflux value. From the McCabe-Thiele method, it was determined that 19 theoretical stages is required (including reboiler), and a minimum reflux of 2.82 was found. This minimum reflux value seemed more reasonable than the one found using the FUG method, and was therefore used in all the following calculations.

Once the minimum reflux ratio was determined, it was possible to show the relationship between the number of trays and the reflux ratio as shown in Figure 3. The reflux ratio in Figure 3 is based on the minimum reflux ratio calculated using the McCabe-Thiele method.

![Figure 3: Number of Theoretical Stages as a Function of Reflux Ratio](image)

Figure 3: Number of Theoretical Stages as a Function of Reflux Ratio

Figure 3 provides a rough estimate for the number of stages at a given reflux ratio. The optimum point should be taken where the capital cost and the operating costs are balanced, where the capital costs are dependent on the number of trays and the operating costs are based on the reflux ratio. From Figure 3, a reflux ratio of 3.7 was chosen. At this reflux ratio, 10.35 trays are required. This number of trays is expected to increase once the tray efficiency is determined and will be discussed in later sections.
After determining the number of trays required for the distillation column, the next step in the design procedure is to decide which type of tray is best suited for the tower – based on cost and efficiency.

**Tray Type Selection**

Distillation towers commonly use bubble-cap trays, sieve trays, valve trays, or dual-flow trays depending on the separation process. Figure 4 shows the market presence of the various types of trays and since no information was found for dual-flow trays its market presence was assumed to be minimal.

![Figure 4: Market Share of Tray Types](image)

Figure 4 shows that valve trays are one of the more popular tray types to use in distillation towers, but a decision on the type of tray should not be based on this alone. An extensive comparison of the different tray types was performed in order to reach a decision on the best tray for the acetone-water distillation tower. Table 3 summarizes some of the key points that were considered in choosing the tray type (Kister, 1992):
Table 3: General Comparison of Tray Types

<table>
<thead>
<tr>
<th>Type</th>
<th>Bubble-Cap Tray</th>
<th>Sieve Tray</th>
<th>Valve Trays</th>
<th>Dual-Flow Trays</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Capacity</strong></td>
<td>Moderately High</td>
<td>High</td>
<td>High to Very High</td>
<td>Very High</td>
</tr>
<tr>
<td><strong>Pressure Drop</strong></td>
<td>High</td>
<td>Moderate</td>
<td>Moderate</td>
<td>Low to moderately</td>
</tr>
<tr>
<td><strong>Efficiency</strong></td>
<td>Moderately High</td>
<td>High</td>
<td>High</td>
<td>Low compared to others</td>
</tr>
<tr>
<td><strong>Cost</strong></td>
<td>High – approximately 2 to 3 times more expensive than sieve trays</td>
<td>Low</td>
<td>~ 20% more expensive</td>
<td>Low</td>
</tr>
<tr>
<td><strong>Maintenance Requirements</strong></td>
<td>Relatively High</td>
<td>Low</td>
<td>Low to Moderate</td>
<td>Low</td>
</tr>
<tr>
<td><strong>Fouling Tendency</strong></td>
<td>High. Tends to collect solids.</td>
<td>Low</td>
<td>Low to Moderate</td>
<td>Extremely low</td>
</tr>
<tr>
<td><strong>Effects of Corrosion</strong></td>
<td>High</td>
<td>Low</td>
<td>Low to Moderate</td>
<td>Very low</td>
</tr>
</tbody>
</table>

Some of the key parameters that affect the choice of the tray type are cost, the efficiency of the tray, and the overall maintenance requirements. Other important parameters that were considered in the selection process were turndown ratio, amount of entrainment, and overall complexity of the tray.

In consideration of the above factors for designing a distillation column, the valve tray seems to be the best suited tray type for the separation of acetone-water. A graphical representation of a valve tray has been included in Figure 5. It has a low cost relative to the other types, requires a small amount of maintenance, has the capacity to handle high flow rates, and is highly efficient. Valve trays also account for approximately 70% of all tray types, and can handle a turndown ratio of approximately 4-5 to 1. Even though a variable load is not expected in the phenol plant, the use of valve trays would be a preemptive approach since even a short
turndown period can result in high energy costs. The higher capital costs of valve trays may be negligible if faced with higher energy costs in a turndown situation (Kister, 1992). After determining the type of tray, it is important to consider the efficiency of the trays.

![Figure 5: Simple Valve Tray](image)

**Tray Efficiency**

The tray efficiency for the acetone-water distillation column was determined using an empirical formula from O’Connell. The correlation was originally formulated for bubble-tray towers, but it also suitable for valve trays where predictions will be slightly conservative (Geankoplis, 2003). Using this correlation the overall tray efficiency was determined to be approximately 0.59. For this tray efficiency the actual number of trays required for the distillation column is 18 stages. Calculations for the tray efficiency and the actual number of trays have been summarized in Appendix C.

**Tray Spacing**

Another important parameter to consider when designing any distillation column is the distance between the trays, or tray spacing. The tray spacing is often dependent on whether the system is operated under vacuum conditions, moderate to high pressures, or at atmospheric. Towers that operate under vacuum conditions often are spaced between 0.61 to 0.76m apart, while atmospheric distillation columns tend to be between 0.31 and 0.76m apart. For the acetone-water distillation tower a tray spacing of 0.457m (or 18 inches) will be used (Chopey, 2003). After determining the tower diameter, the tray spacing was verified using a correlation (Thibault, 2010) and the actual tray spacing was determined to be 0.600m (or 24 inches). These calculations have been provided in Appendix C.
Column Diameter and Height

Once the tray spacing and the number of trays have been determined for the column, it is possible to calculate the diameter and height of the tower, once the flooding velocity is known. The height is dependent on the number of trays, the spacing required for the trays, and extra space to accommodate manholes, feed and side-streams arrangements, and interpolate cooling (Thibault, 2010).

The flooding velocity was determined using correlations and it was found to be approximately 1.4 m/s. Using this value and accounting for the downcomer area, the diameter of the tower was calculated to be approximately 1.83 m. After recalculating the tray spacing using correlations (Thibault, 2010), the column height was calculated to be approximately 12.95m. This height includes 1.22m at the top to minimize entrainment and account for extra spacing for manholes, and 1.53m at the bottom for the reboiler (Geankoplis, 2003). Once these values have been finalized, the design of the distillation column is almost complete. The next step is to determine the auxiliary equipment required for the distillation column.

Other Equipment

Other equipment required for the operation of a distillation tower includes the condenser, reboiler, reflux drum, and the reflux pump and motor. Some of the key design parameters for this equipment have been summarized in the Table 4. The cost for this equipment has been summarized in Chapter 7.

Table 4: Summary of Auxiliary Equipment

<table>
<thead>
<tr>
<th>Equipment Used</th>
<th>Area/Volume/kWrequired</th>
</tr>
</thead>
<tbody>
<tr>
<td>Condenser</td>
<td>Floating Head Heat Exchanger</td>
</tr>
<tr>
<td>Reboiler</td>
<td>Kettle Reboiler</td>
</tr>
<tr>
<td>Reflux Drum</td>
<td>Horizontal Process Vessel</td>
</tr>
<tr>
<td>Reflux Pump</td>
<td>Centrifugal Pump</td>
</tr>
</tbody>
</table>
The equipment listed in Table 4 is essential to the operation of the distillation column. The condenser is used to condense the final vapor product. Some of the condensed liquid product, or distillate, is removed. The remaining liquid from the condenser is then returned, or refluxed, as a liquid to the top tray of the column. This helps achieve a high purity in the distillate stream. The reboiler is necessary for partially vaporizing the liquid leaving the bottom tray. The remaining liquid which is lean in acetone is withdrawn as the bottoms product and sent to the wastewater treatment facility. The reboiler also helps to achieve a high recovery of acetone. The reflux drum and reflux pump form part of the condenser since the condenser will be located at ground level, and not above ground as usually depicted in distillation column graphics.

For the condenser, the cooling water will enter at a temperature of 20°C and leave at no more than 35°C (based on fall conditions). The condenser requires approximately $4.3 \times 10^4$ kg/h of water. The reboiler will use low pressure saturated steam at 120°C and approximately 2 bars (Thibault, 2010). The steam requirement is approximately 1200 kg/h.

The final step of the design of distillation columns can now be completed, which is choosing the materials of construction.

**Materials of Construction**

The choice of materials of construction is an extremely important step in the design of distillation towers, as it affects the safety of the process and also the capital costs. In consideration of this, the following factors should be examined when choosing a particular material for construction (Coulson, 2003):

- Mechanical Properties (i.e., strength, wear resistance)
- Effect of temperature on the mechanical properties
- The materials resistance to corrosion
- Ease of fabrication
- The availability of the material particularly in the desired size
- Cost
In the separation of acetone and water via a distillation column, there are no inherent corrosion concerns. Therefore, the material of construction does not necessarily need to resist corrosion, and for this reason, carbon steel was an ideal choice for the tower and also the trays.

Figure 6 compares the relative cost of carbon steel and other materials of construction for trays (Kister, 1992). These relative costs of materials will likely represent the costs involved for other pieces of equipment too, including the column vessel, reboiler, condenser, and reflux drum materials. Using carbon steel as the material of construction for all of these pieces of equipment will result in significant capital cost savings.

![Figure 6: Relative Tray Costs as a Function of Construction Material](image)

Once the material of construction has been chosen for the distillation column and auxiliary equipment, it is now possible to determine the costs involved. This has been summarized in Chapter 7.
Table 5: Summary of Distillation Column

<table>
<thead>
<tr>
<th></th>
<th>Distillation Column T-402</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Theoretical Trays</td>
<td>10.35</td>
</tr>
<tr>
<td>Type of Trays</td>
<td>Valve Tray</td>
</tr>
<tr>
<td>Overall Efficiency of Trays</td>
<td>0.588</td>
</tr>
<tr>
<td>Number of Actual Trays</td>
<td>18</td>
</tr>
<tr>
<td>Tray Spacing</td>
<td>0.600m*</td>
</tr>
<tr>
<td>Material of Construction</td>
<td>Carbon Steel</td>
</tr>
<tr>
<td>Operating Pressure</td>
<td>101.325 kPa</td>
</tr>
<tr>
<td>Operating Temperature</td>
<td>~60 °C</td>
</tr>
</tbody>
</table>

*Initial estimate was 0.457m, but it was later determined to be 0.600m

Table 5 summarizes some of the important design specifications for the acetone-water distillation column required for the phenol plant. The above design for the acetone-water distillation column was implemented in UniSim and gave reasonable results. The desired purity of acetone was 99.5% (by weight), and UniSim was returning values of 99.4% (by weight) for a reflux ratio of 3.7.
Chapter 6: Environmental/Safety Considerations

Some of the safety considerations that should be considered in the design and operation of a distillation column include: prevent the tower from reaching high pressures, the presence of manholes for column access, and proper waste treatment.

Distillation towers, as well as other towers and drums, must be protected from any overpressure that may occur as a result of malfunction, fire or utility failure (Stellman, 1998). Important measures must be employed in order to develop a process safety strategy that will improve safety, minimize any losses, and also protect the workers health. The proper way to protect against overpressure in distillation towers is by using pressure relief valves. Often the pressure relief valve is located near the top of the tower to handle the vapour load, but there have been towers where different locations have been used for the pressure relief valves (Stellman, 1998). Basically how a pressure relief valve works is by discharging to the atmosphere or a closed system. If it is decided that the discharge should be to the atmosphere, then it is imperative to determine whether this discharge may potentially put the workers health at risk or not.

Another safety concern for distillation towers is the presence of manholes for column access. These manholes are essential for cleaning any fouling that may occur within the column, and the number of manholes is often dependent on the number of trays. There should be at least one manhole per 30 trays in a clean and noncorrosive column (Kister, 1990). When the maintenance crew are entering the manholes for cleaning, they should wear the appropriate personal protective equipment (PPE) and have previously completed the confined spaces training offered by C2P Design.

Other considerations for the maintenance crew working within the confines of the distillation column include:
- Check their safety equipment before entering the column
- Ensure that workers are aware of any hazards present within the column
- Be confident that the column is safe for entry
- Ensure that a worker is stationed outside the column in case the maintenance worker inside the column is injured

Also, if it is deemed necessary that a damaged tray be removed and replaced then special safety requirements should be upheld in order to protect the maintenance worker. Often, sharp pieces of metal from the trays can be left hanging, or may become brittle and therefore not support the worker’s weight (Kister, 1992).

Finally, the water that is separated in tower T-402 is eventually sent to a wastewater treatment facility, as it will contain trace amounts of acetone. A common regulatory limit for acetone is 6.3 mg/L (Web-1, 2010), and therefore the wastewater should aim to meet this limit or aim for even lower as it may pose environmental risks.
Chapter 7: Capital Estimate

Separations form an integral part of most processing plants. The importance of recovering high purity products helps justify the fact that separation units constitute a major percentage of the plant’s capital investment, and contribute significantly to the total energy consumption. On average, separation equipment accounts for 40-50% of the total capital cost, and 70% of the total energy consumption. Of that 70%, 95% of this energy consumption is attributed to distillation columns (Chen, 2001). These numbers prove that extreme care should be taken in the economic analysis of distillation towers to help minimize costs – both operating and capital.

Distillation towers can often have substantial capital costs where these costs are usually dictated by the following factors:

- Tray Types
- Materials of Construction
- Column diameter/height
- Condenser/Reboiler
- Reflux Pump + Motor
- Reflux Drum

The costs for the column/trays and any auxiliary equipment has been calculated using correlations provided by Turton. Figure 7 summarizes the contribution of all the equipment associated with the distillation column to the overall capital cost. It is easy to recognize that the distillation vessel itself invokes the majority of costs, or approximately 31%. The other major contributors to the cost include the valve trays and the condenser, where the condenser is modeled as a floating head heat exchanger. The total cost of the distillation column and its auxiliary equipment is approximately $470,000, and has been corrected using a CEPCI of 521.9 for 2009. Even though the cost is estimated at $470,000 for the distillation column, often in new developments (or grassroots facilities) there is extra cost involved for constructing on undeveloped land. For this particular piece of equipment, the grassroots cost is approximately $790,000.
Some of the parameters that influence the cost of the column include the diameter, height of column, type of construction material, thickness of wall, and several others. Figure 8 shows how the cost of the column would increase substantially with increases in the diameter.

**Figure 7: Cost Comparison of Major Equipment**

**Figure 8: Bare Module Costs for Column and Trays as a Function of Diameter**
The diameter of the column not only affects the bare module cost of the column, where an increase in diameter would increase the vessel’s volume, but it also affects the cost of the trays. It affects the cost of the tray since the area of the tray is dictated by the diameter of the column. From Figure 8 it can be seen that the cost of the trays does not rise as quickly as the cost of the column with an increase in diameter. The diameter also affects the spacing of the trays, which could result in an increase in height, and therefore an increase in cost. For this reason, it was imperative to design a distillation column as to minimize the diameter and minimize the capital costs involved.

![Figure 9: Capital Cost of Plant as a Function of Reflux Ratio](image)

Figure 9 shows that the reflux ratio is essential in determining the capital cost of the distillation column, and is based on the assumption that the column and the trays dictate the capital cost of the distillation column. It can be seen that at smaller reflux ratio that the capital costs are significantly higher. At a lower value for reflux ratio, the number of trays increases, along with the height of the column which both contribute to larger capital costs. One important thing to note about Figure 9 is that the operating costs will increase as the reflux ratio increases, as more utilities will be required. The operating costs associated with the distillation column could be minimized with heat integration, if it was possible to match a hot stream for use in the reboiler, or match cold streams in the condenser. The heat integration could possible reduce
the demand for cooling water or low pressure saturated steam. Once the operating costs have been determined, it will be possible to determine the optimum design of the distillation column.

Other considerations which may increase the capital costs of the distillation column significantly, is the material of construction. For the acetone-water separation, the column does not need to account for any corrosion. The column also does not operate at extreme conditions, and therefore is capable of using carbon steel as its material of construction. The trays, reflux drum, reboiler, and condensers can also all be made from carbon steel. Figure 10 compares the capital cost using carbon steel as opposed to stainless steel or a nickel alloy.

Figure 10: Comparison of Plant Cost Using Different Materials of Construction

After a review of the capital costs involved in the separation of acetone-water using a distillation column, it is evident that it is a costly venture. The total cost of the tower approaches $470,000. Before determining whether other possible routes of separation should be researched, an extensive study will have to be performed on the operating costs involved with this tower. As mentioned previously, the operating costs will largely be affected by the reflux ratio.
References


Web References

Appendix C: Sample Calculations

C-1: Design Calculations for Distillation Columns

FUG Method
The Fenske-Underwood-Gilliland (FUG) method is a shortcut method which provides an initial estimate of the reflux ratio, number of equilibrium stages, and location of the feed stage. Details on the calculation are presented below for Tower T-402.

1. Fenske Relation for Minimum Number of Stages

The Fenske relation for the minimum number of stages in a plate column is given by:

\[ N_{\text{min}} = \frac{\log\left(\frac{X_{\text{LK}}}{X_{\text{HK}}} \cdot \frac{X_{\text{HK}}}{X_{\text{LK}}} \middle/ \frac{X_{\text{LK}}}{X_{\text{HK}}}\right)}{\log\alpha^{\text{ave}}_{\text{LK}/\text{HK}}} \]  

Where:

- \( N_{\text{min}} \) = minimum number of plates required (total reflux)
- \( X_{\text{LK}} \) = molar fraction of the light key component (-)
- \( X_{\text{HK}} \) = molar fraction of the heavy key component (-)
- \( \alpha \) = relative volatility (-)

The subscripts B and D refer to the bottoms and distillate, respectively.

The key components refer to those between which it is desired to make the separation. In Tower T-402, the key components are water and acetone. The light key component is the one that is desired to be kept out of the bottom product, while the heavy key component is to be kept out of the top product. The assumption is also made that all
components lighter than the light key go entirely in the distillate and those heavier than the heavy key go to the bottoms.

To solve for the average relative volatility in equation (1), the following expression can be used:

$$\alpha_{L_{K}/H_{K}}^{Ave} = \left(\frac{\alpha_{L_{K}/H_{K}}^D \alpha_{L_{K}/H_{K}}^B}{1/2}\right)$$ (2)

The relative volatility of the components can be found using the relation:

$$\alpha_{L_{K}/H_{K}} = \frac{\left(\frac{y_{L_{K}}}{x_{L_{K}}}\right)}{\left(\frac{y_{H_{K}}}{x_{H_{K}}}\right)}$$ (3a)

Where: $y =$ molar fraction in the vapour phase (-)

$x = molar$ fraction in the liquid phase (-)

The K-value is a useful quantity which can be used in relative volatility calculations. It is defined as:

$$K_i = \frac{y_i}{x_i}$$ (4)

Where the subscript $i$ refers to the $i^{th}$ component.

Using K-values, the relative volatility can be re-expressed:

$$\alpha_{L_{K}/H_{K}} = \frac{K_{L_{K}}}{K_{H_{K}}}$$ (3b)
To illustrate the calculation, the relative volatility of the light key to the heavy key in the bottoms is computed. The compositions are taken from the UniSim simulation, and acetone is the light key and water is the heavy key.

Calculating K-values using equation (4):

\[ K_{LK,D} = \frac{y_{acetone,D}}{x_{acetone,D}} \]  

\[ K_{LK,D} = \frac{0.9843}{0.9841} \]

\[ K_{LK,D} = 1 \]

\[ K_{LK,D} = \frac{y_{water,D}}{x_{water,D}} \]  

\[ K_{LK,D} = \frac{0.0137}{0.0159} \]

\[ K_{LK,D} = 0.862 \]

Using these K-values, the relative volatility in the distillate can be calculated:

\[ \alpha_{LK,HK} = \frac{1.0003}{0.862} \]  

\[ \alpha_{LK,HK} = 1.16 \]

Similarly, the compositions in the bottoms were used to calculate the relative volatility of LK/HK here. The resulting value is:

\[ \alpha_{LK/HK,B} = 3.21 \]
Substituting these values to find the average relative volatility (equation 2):

\[ \alpha_{\text{KL}/\text{HK}}^{\text{Ave}} = (1.16 \times 3.21)^{1/2} \]

\[ = 1.92 \]

Using this value and compositions of the key components as extracted from UniSim, the minimum number of plates can be estimated using equation (1):

\[ N_{\text{min}} = \frac{\log \left( \frac{0.9814}{0.0159} \times \frac{0.3119}{0.6832} \right)}{\log 1.92} \]

\[ = 5.12 \text{ [stages]} \]

2. Underwood Equations for Minimum Reflux Ratio

The minimum reflux ratio can be calculated using the follow two equations proposed by Underwood (1946):

\[ \sum_{i=1}^{n} \frac{\alpha_i x_{i,F}}{\alpha_i - \theta} = 1 - q \quad (5) \]

\[ R_{\text{min}} + 1 = \sum_{i=1}^{n} \frac{\alpha_i x_{i,D}}{\alpha_i - \theta} \quad (6) \]

Where: \( \theta = \) Underwood constant \((1 < \theta < \alpha_{\text{KL}})\)

\( x_{i,F} = \) mole fraction in the feed

\( q = \) feed thermal quality \((\text{fraction liquid})\)

\( R_{\text{min}} = \) minimum reflux ratio

And the index represents the components i through n components present.
The Underwood constant can be found using an iterative procedure in equation (5). The relative volatilities of each component in the feed were used for the calculation of the summation in equation (5). Rearranging equation (5):

\[ q = 1 - \sum_{i=1}^{n} \frac{\alpha_i x_{i,F}}{\alpha_i - \theta} \quad (5) \]

Knowing that the feed quality is 1 for saturated liquids, iterations can be performed at different values of \( \theta \) until equation (5) converges. This was done using Microsoft Excel and the value of \( \theta = 1.192 \) was obtained.

Once this value was found, the minimum reflux ratio was then estimated using equation 6:

\[ R_{min} = \sum_{i=1}^{n} \frac{\alpha_i x_{i,D} \theta}{\alpha_i - \theta} - 1 \quad (6) \]

\[ = 1.4832 - 1 \]

\[ = 0.4832 \]

The optimum reflux ratio was taken as 1.4 times the minimum reflux ratio. This is taken from heuristics (Thibault, 2010).

In this case:

\[ R_{opt} = 0.4832 \times 1.4 \]

\[ = 0.676 \]
3. Gilliland Equation for Number of Equilibrium Stages

The Gilliland equation for number of equilibrium stages $N$ as a function of the minimum number of stages ($N_{min}$), the minimum reflux ratio ($R_{min}$), and the operating reflux ratio ($R$). The equation is as follows:

$$\frac{N - N_{min}}{N + 1} = 0.75 \left[ 1 - \left( \frac{R - R_{min}}{R + 1} \right)^{0.566} \right] \quad (7)$$

Where: $N = \text{number of equilibrium stages}$

$R = \text{actual reflux ratio}$

The number of equilibrium stages can be calculated using the calculated minimum reflux ratio and calculated minimum number of stages, as well as assuming that $R = R_{opt}$, as calculated.

Substituting values for T-402:

$$\frac{N - 5.12}{N + 1} = 0.75 \left[ 1 - \left( \frac{0.676 - 0.4832}{0.676 + 1} \right)^{0.566} \right] \quad (7)$$

$$\frac{N - 5.12}{N + 1} = 0.529457$$

$$N - 5.12 = 0.529457N + 0.529457$$

$$0.4705N = 5.649457$$

$$N = \textbf{12 stages}$$
McCabe-Thiele Method

Another method used for the design of the distillation tower included the McCabe-Thiele method, which is a graphical method for solving the equilibrium relationship. For binary distillation, the McCabe-Thiele method assumes that the feed is a saturated vapor and that the distillation operates with a total condenser. Other assumptions for using this method are that the separation occurs at constant pressure. This assumption usually holds true for distillation columns not operating under vacuum conditions.

When using the McCabe-Thiele method it is important to consider the following three items:

1. Constant Molar Overflow Assumption
2. Operating Line
3. Equilibrium Curve

The constant molar overflow assumption implies the following:

- Molal heats of vaporization of the components are roughly the same
- Heat effects (heats of solution, heat losses to and from column, etc) are negligible
- For every mole of vapour condensed, one mole of liquid is vaporized

The first step in the McCabe-Thiele method is to plot the x-y diagram, which represents the vapour-liquid equilibrium (VLE) data. On this plot, any point on the curve represents the amount of liquid that is in equilibrium with vapour at different temperatures. The VLE plot for the acetone-water separation is shown in Figure 11.
Figure 11: Acetone-Water VLE Data

Once the VLE data for the lower-boiling point component has been plotted, the next step of the McCabe-Thiele procedure can be performed.

A straight line is drawn from the origin to the point where the mole fraction of acetone in the liquid and vapour phases is equal to 1 (i.e., where y and x equal 1). The straight line is essentially a 45 degrees line to aid for drawing the operating lines.

The next step is to draw the q line. The slope of the q line is slightly above one meaning that the feed is a slightly subcooled liquid feed. The q line is colored with a thick blue line as indicated in Figure 12. Other lines are also plotted, including the operating lines for the enriching section and the stripping section, both of which are labeled in Figure 12.
The equation for the **q line** is as follows:

\[ y = \frac{q}{q-1} x - \frac{x_F}{q-1} \]

Where,

\[ q = \frac{H_v - H_f}{H_v - H_L} \] and \( H_v \) is the enthalpy of the feed, \( H_L \) the enthalpy of the feed at the boiling point, and \( H_f \) is the enthalpy of the feed at its entrance condition.

The equation for the **enriching operating line** is as follows:

\[ y_{n+1} = \frac{R}{R + 1} x_n + \frac{x_D}{R + 1} \]

Where,

\[ R = \text{Reflux Ratio} \]
\[ x_D = \text{mole fraction at distillate} \]

And, for the **stripping operating line**:

\[ y_{m+1} = \frac{L_m}{V_{m+1}} x_m + \frac{W x_W}{V_{m+1}} \]

From Figures 12 and 13 it is evident that 19 equilibrium stages for the acetone-water distillation column was found using the McCabe-Thiele Method. If you subtract one stage for the reboiler, then the total theoretical trays is 18 for the McCabe-Thiele method.
Figure 12: McCabe-Thiele Method (Part 1)
Figure 13: McCabe-Thiele Method (Part 2)
Other calculations required for the design of distillation columns are as follows:

The flooding velocity (m/s) can be calculated using the following equation:

\[ U_{max} = K_v \left( \frac{\sigma_L}{20} \right)^{0.2} \sqrt{\frac{\rho_L - \rho_G}{\rho_G}} \]

Where,

- \( K_v \) = a correction factor that is estimated (Geankoplis, 2003)
- \( \sigma_L \) = liquid surface tension \( \text{dyne/cm} \)
- \( \rho_L \) = the density of the liquid
- \( \rho_G \) = the density of the vapour

Applying these values to the above equation, we find:

\[ U_{max} = K_v \left( \frac{\sigma_L}{20} \right)^{0.2} \sqrt{\frac{\rho_L - \rho_G}{\rho_G}} = \left( \frac{0.29 \text{ ft/s}}{1 \text{ ft}} \right) \times \frac{0.3048 \text{ m}}{1 \text{ ft}} \times 0.91 \times \left( \frac{33.16}{20} \right)^{0.2} \sqrt{\frac{769.2 - 2.022}{2.022}} \]

\[ = 1.733 \text{ m/s} \]

Note: The value of \( K_v \) was estimated at 0.29 from Geankoplis. \( K_v \) should be multiplied by 0.91 to account for a downspout area of 9% of the tray (Geankoplis, 2003). This plot has been provided in Figure 14.
Figure 14: Estimation of Kv Value for Allowable Vapor Velocity

Also, the Umax should be multiplied by 0.80 in order to operate at 20% below flooding.

\[ U_{max} = (0.8) \times 1.733 = \frac{1.39 \, m}{s} \]

The flooding velocity for Tower T-402 is 1.39 m/s.

The tower diameter (m) can be calculated using the following equation:

\[
D_T = \sqrt{\frac{4G}{(fU_f)\pi \left(1 - \frac{A_d}{A_T}\right) \rho_G}}
\]

Where,

\[
\frac{A_d}{A_T} = \begin{cases} 
0.1 + \frac{F_{LV} - 0.1}{9} & \text{for } F_{LV} \leq 0.1 \\
0.2 & \text{for } 0.1 \leq F_{LV} \leq 1.0 \\
& \text{for } F_{LV} \geq 1.0
\end{cases}
\]

And,

\[
F_{LV} = \frac{L_m}{V_m} \sqrt{\frac{\rho_v}{\rho_L}}
\]
Applying values to the above equations, we find,

\[
\frac{A_d}{A_T} = 0.1 + \frac{F_{LV} - 0.1}{9} = 0.1 + \frac{0.055778 - 0.1}{9} = 0.095086
\]

\[
F_{LV} = \frac{L_m}{V_m} \sqrt{\frac{\rho_v}{\rho_L}} = \frac{415.8}{382.2} \sqrt{\frac{2.022}{769.2}} = 0.055778
\]

\[
D_T = \sqrt{\frac{4G}{(fU_f)\pi}} \left(1 - \frac{A_d}{A_T}\right) \rho_g = \sqrt{\frac{4(19320) \cdot \frac{1}{3600}}{(0.8) \cdot 1.39)\pi(1 - 0.095086)(2.022)}} = 1.83m
\]

The diameter of the distillation column is 1.83 m.

Using this value we can check our initial estimate of the tray spacing.

\[
H_p = 0.5 \cdot (D)^{0.3} = 0.5 \cdot (1.83)^{0.3} = 0.600m
\]

This value is relatively close to our previous estimation and should not affect the value of Kv significantly; therefore the values obtained via the above calculations should be similar.

Overall Efficiency of Tray Towers

\[
E_o = 0.492 \cdot (\mu_L \alpha)^{-0.245}
\]

If we apply values to the above equation, we find,

\[
E_o = 0.492 \cdot (\mu_L \alpha_{ave})^{-0.245} = 0.492 \cdot (0.2546 \cdot 1.90)^{-0.245} = 0.588
\]

If the overall efficiency of our tower is 0.588, then it is now possible to determine the total number of trays required:

\[
E_o = \frac{\text{# of ideal trays}}{\text{# of actual trays}}
\]

If we rearrange the above equation, it is possible to calculate the actual # of trays:
Height of the Column

The height of the column is dependent on the number of trays, tray spacing, and some additional space to minimize entrainment and account for the reboiler height.

\[
\text{Height of Column} = (N_{\text{actual}} - 1) \times H_p + \sum \Delta H
\]

Plugging values into the above equation, we arrive at,

\[
\text{Height of Column} = (18 - 1) \times .6 + (1.22 + 1.53) = 12.95 \text{ m}
\]

Note: The height of the column assumes a height of 1.22 m to minimize entrainment, and 1.53 m for the reboiler (this calculation is shown later).
C-2: Costing Calculations

The values used in the calculations below have been extracted from Turton et Al, 2009.

**Distillation Column**

**Thickness for Cylindrical Vessels**

\[ t = \frac{PR}{0.9S - 0.6P} + t_c \]

Where,

- \( P = \) internal pressure, bar
- \( t = \) wall thickness, m
- \( t_c = \) additional allowance for corrosion, \(~0.003\) m
- \( S = \) allowable tensile stress, bar
- \( R = \) internal radius, m

The allowable tensile stress for carbon steel between temperatures of -200 to 450°C is approximately 960 bar which can be used in the above equation.

Applying values to the above equation, we find:

\[ t = \frac{PR}{0.9S - 0.6P} + t_c = \frac{(1.01325)(0.915)}{0.9(960) - 0.6(1.01325)} + 0.003 = 0.00407 \text{ m} \]

**Pressure Factor for Distillation Column,**

\[ F_{P,vessel} = \frac{(P + 1)D}{2[850 - 0.6(P + 1)]} + 0.00315 \quad \text{for } t_{vessel} > 0.0063 \text{ m} \]

In the above equation if \( F_{P,vessel} \) is less than 1 (corresponding to \( t_{vessel} < 0.0063 \) m), then \( F_{P,vessel} \) is equal to 1.

For the acetone-water separation tower, the \( F_{P,vessel} \) is equal to 1 since the thickness of the vessel is less than 0.0063m.
**Purchase Cost of Distillation Column (assuming a vertical vessel),**

\[ \log_{10} C_P^o = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2 \]

For **process vessels**, the following values apply:

\[ K_1 = 3.4974 \]
\[ K_2 = 0.4485 \]
\[ K_3 = 0.1074 \]
\[ A = 34.85 \text{ m}^3 \]

Applying these values to the above equation, we find:

\[ \log_{10} C_P^o = 3.4974 + (0.4485)\log_{10}(34.06) + (0.1074)[\log_{10}(34.06)]^2 = 4.437 \]

\[ C_P^o = 10^{4.437} = 27353 \]

**Bare Module Cost for Process Vessel**

\[ C_{BM} = C_P^o F_{BM} = C_P^o (B_1 + B_2 F_M F_P) \]

For **process vessels** the following values apply,

\[ B_1 = 2.25 \]
\[ B_2 = 1.82 \]
\[ F_M = 1 \]
\[ F_P = 1 \text{ (from above)} \]

Applying these values to the above equation, we find:

\[ C_{BM} = C_P^o F_{BM} = C_P^o (B_1 + B_2 F_M F_P) = (27353)(2.25 + (1.82)(1)(1)) = 111327 \]

If we correct for the CEPCI values then,

\[ C_{BM}^o = 111327 \left( \frac{521.9}{397} \right) = 146352 \]
Valve Trays

**Purchase Cost of valve trays,**

\[
\log_{10} C_p^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2
\]

\[
K_1 = 3.3322
\]

\[
K_2 = 0.4838
\]

\[
K_3 = 0.3434
\]

\[
A = 2.6302 \text{ m}^2
\]

Applying these values to the above equation, we find:

\[
\log_{10} C_p^0 = 3.3322 + (0.4838) \log_{10}(2.6302) + (0.3434) [\log_{10}(2.6302)]^2 = 3.596
\]

\[
C_p^0 = 10^{3.596} = 3944
\]

**Bare Module Cost for Valve Trays**

\[
C_{BM} = C_p^0 NF_{BM} F_q
\]

Where,

\[
F_{BM} = 1 \text{ (taken from Figure A.19 from Turton)}
\]

\[
F_q = 10^{0.4771 + 0.08516 \log_{10}(18) - 0.3473(\log_{10}(18))^2} = 1.088
\]

The above equation for \( F_q \) applies only if the number of trays in the column is below 20. If the columns exceed 20, then \( F_q \) is equal to 1.

Applying values to the equation for valve trays above, the base module cost for the valve trays is as follows:

\[
C_{BM} = C_p^0 NF_{BM} F_q = (3944)18(1)(1.088) = 77239
\]

If we correct for the CEPCI values then,

\[
C_{BM}^o = 77239 \left(\frac{521.9}{397}\right) = 101539
\]
Condenser
The condenser is assumed to operate as a floating head heat exchanger.

**Purchase Cost of condenser,**

\[ \log_{10} C^o_p = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2 \]

For the condenser (assuming it’s a floating head heat exchanger), the following values apply:

\[ K_1 = 4.8306 \]
\[ K_2 = -0.8509 \]
\[ K_3 = 0.3187 \]
\[ A = 34.6 \, m^2 \]

Applying these values to the above equation, we find:

\[ \log_{10} C^o_p = 4.8306 + (-0.8509)\log_{10}(34.6) + (0.3187)[\log_{10}(34.6)]^2 = 4.2759 \]

\[ C^o_p = 10^{4.2759} = $18877 \]

**Bare Module Cost for the Condenser,**

\[ C_{BM} = C^o_p F_{BM} = C^o_p (B_1 + B_2 F_M F_P) \]

For condensers (assuming a floating head heat exchanger) the following values apply,

\[ B_1 = 1.63 \]
\[ B_2 = 1.66 \]
\[ F_M = 1.4 \]

\[ F_P = 10^{C_1+C_2\log_{10}(P)+C_3(\log_{10}P)^2} = 10^{0+0\log_{10}(P)+0(\log_{10}P)^2} = 10^0 = 1 \]
Applying these values to the above equation, we find:

\[ C_{BM} = C^0_p F_{BM} = C^0_p (B_1 + B_2 F_M F_P) = (18877) (1.63 + (1.66)(1.4)(1)) = 74640 \]

If we correct for the CEPCI values then,

\[ C^0_{BM} = 74640 \left( \frac{521.9}{397} \right) = 98122 \]
Reboiler
The reboiler is assumed to operate as a kettle reboiler.

**Purchase Cost of reboiler,**

\[
\log_{10} C_P^o = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2
\]

For the reboiler (assuming it’s a kettle reboiler), the following values apply:

\[
\begin{align*}
K_1 &= 4.4646 \\
K_2 &= -0.5277 \\
K_3 &= 0.3955 \\
A &= 13.13 m^2
\end{align*}
\]

Applying these values to the above equation, we find:

\[
\log_{10} C_P^o = 4.4646 + (-0.5277)\log_{10}(13.13) + (0.3955)[\log_{10}(13.13)]^2 = 4.369
\]

\[
C_P^o = 10^{4.369} = $23388
\]

**Bare Module Cost for the Reboiler**

\[
C_{BM} = C_P^o F_{BM} = C_P^o (B_1 + B_2 F_M F_P)
\]

For the reboiler (assuming a kettle reboiler) the following values apply,

\[
\begin{align*}
B_1 &= 1.63 \\
B_2 &= 1.66 \\
F_M &= 1 \\
F_P &= 10^{C_1 + C_2 \log_{10}(P) + C_3 (\log_{10}(P))^2} = 10^{0 + 0 \log_{10}(P) + 0 (\log_{10}(P))^2} = 10^0 = 1
\end{align*}
\]

Applying these values to the above equation, we find:

\[
C_{BM} = C_P^o F_{BM} = C_P^o (B_1 + B_2 F_M F_P) = (23388)(1.63 + (1.66)(1)(1)) = $76947
\]

If we correct for the CEPCI values then,

\[
C_{BM}^{o} = $76947 \left( \frac{521.9}{397} \right) = $101155
\]
Reflux Drum

For the reflux drum (horizontal process vessel),

**Purchase Cost of reflux drum,**

\[
\log_{10} C_P^0 = K_1 + K_2 \log_{10} (A) + K_3 [\log_{10} (A)]^2
\]

For the reflux drum (assuming it’s a horizontal process vessel), the following values apply:

\[
K_1 = 3.5565 \\
K_2 = 0.3776 \\
K_3 = 0.0905
\]

\[A = 1.681 \text{ m (length)}\]

Applying these values to the above equation, we find:

\[
\log_{10} C_P^0 = 3.5565 + (0.3776)\log_{10}(1.681) + (0.0905)[\log_{10}(1.681)]^2 = 4429
\]

**Pressure Factor for Horizontal Process Vessel**

\[
F_{P,\text{vessel}} = \frac{(P + 1)D}{2[850 - 0.6(P + 1)] + 0.00315} \quad \text{for } t_{\text{vessel}} > 0.0063 \text{ m}
\]

In the above equation if \(F_{P,\text{vessel}}\) is less than 1 (corresponding to \(t_{\text{vessel}} < 0.0063 \text{ m}\)), then \(F_{P,\text{vessel}}\) is equal to 1.

Since the thickness required for the reflux drum is less than 0.0063, then \(F_p\) is equal to 1.

**Bare Module Cost for the Reflux Drum**

\[
C_{BM} = C_P^0 F_{BM} = C_P^0 (B_1 + B_2 F_M F_p)
\]

For the reflux drum (assuming a horizontal vessel) the following values apply,
Applying these values to the above equation, we find:

\[ C_{BM} = C_p^o F_{BM} = C_p^o (B_1 + B_2 F_M F_P) = 4429 \left( 1.49 + (1.52)(1)(1) \right) = $13331 \]

If we correct for the CEPCI values then,

\[ C_{BM}^o = $13331 \left( \frac{521.9}{397} \right) = $17525 \]
**Reflux Pump + Motor**

The reflux pump will be employed as a centrifugal pump with an electric drive (values extracted from Thibault, 2010).

**Purchase Cost of reflux pump + motor,**

\[ \log_{10} C_P^0 = K_1 + K_2 \log_{10}(A) + K_3 [\log_{10}(A)]^2 \]

For the reflux pump (assuming it’s a centrifugal pump with an electric drive), the following values apply:

\[ K_1 = 3.5793 \]
\[ K_2 = 0.3208 \]
\[ K_3 = 0.002850 \]
\[ A = 0.019879 \text{ kW} \]

Applying these values to the above equation, we find:

\[ \log_{10} C_P^0 = 3.5793 + (0.3208)\log_{10}(0.019879) + (0.002850)[\log_{10}(0.019879)]^2 = 3.04 \]

\[ C_P^0 = 10^{3.04} = \$1096 \]

**Pressure Factor for Reflux Pump**

\[ F_P = C_1 + C_2 \log_{10}(P) + C_3 (\log_{10}(P))^2 \]

Where,

\[ C_1 = 0.1682 \]
\[ C_2 = 0.3477 \]
\[ C_3 = 0.4841 \]
\[ P = 15 \text{ kPa} \]

Applying these values to the above equation,
\[ F_P = C_1 + C_2 \log_{10}(P) + C_3(\log_{10}(P))^2 = 0.1682 + 0.3477 \times \log_{10}(15) + 0.4841(\log_{10}(15))^2 = 1.24673 \]

**Bare Module Cost for the reflux pump with an electric drive**

\[ C_{BM} = C_p^0 F_{BM} = C_p^0 (B_1 + B_2 F_M F_P) \]

For the **reflux pump** the following values apply,

\[
\begin{align*}
B_1 &= 1.80 \\
B_2 &= 1.51 \\
F_M &= 1 \\
F_P &= 1.24673 \text{ (calculated using correlations)}
\end{align*}
\]

Applying these values to the above equation, we find:

\[
C_{BM} = C_p^0 F_{BM} = C_p^0 (B_1 + B_2 F_M F_P) = 1096(1.80 + (1.51)(1)(1.24673)) = 4036
\]

If we correct for the CEPCI values then,

\[
C_{BM}^o = 4036 \left(\frac{521.9}{397}\right) = 5306
\]
**Grassroots Cost**

The grassroots cost refers to a completely new facility in which the construction is done on undeveloped land, such as a grass field (Turton, 2009). In order to determine the grassroots cost, the total module cost is needed first. It can be calculated using the following equation:

\[ C_{TM} = \sum_{i=1}^{n} C_{TM,i} = 1.18 \sum_{i=1}^{n} C_{Bm,i} \]

If we apply numbers to this equation (using the information calculated for each piece of equipment listed above):

\[ C_{TM} = \sum_{i=1}^{n} C_{TM,i} = 1.18 \sum_{i=1}^{n} C_{Bm,i} \]

\[ = 1.18(5306 + 17525 + 101155 + 98122 + 101539 + 146352) = \$554599 \]

From the total module cost, the grassroots cost can be calculated as follows:

\[ C_{GR} = C_{TM} + 0.50 \sum_{i=1}^{n} C_{Bm,i} \]

\[ = \$554599 + 0.50(5306 + 17525 + 101155 + 98122 + 101539 + 146352) \]

\[ = \$789599 \]