

## **Notation**

The most important nomenclature used in this report can be summarized in:

V Vapor flow rate

$V_T$  Vapor flow rate in the top

L Liquid flow rate

D Distillation product

B Bottom product

q Liquid fraction

z Mole fraction in feed

$\alpha$  Relative volatility

$N_C$  number of components

## **Abstract**

Most of the processes in chemical industry are involved in purifying components. As a consequence, a large part of the energy use in many industrial sectors can be attributed to separation processes.

Distillation is the dominant separation technology in chemical industries despite its huge energy consumption. Distillation consumes about 3% of the total energy consumed globally which is equivalent to 2.871.018 J/año [1]

Since many separation tasks need to continue with this technology, methods to determine the minimal energy used in a given distillation task have become important. For separations of a multicomponent mixture, one way to reduce the energy requirements is using thermally coupled distillation columns instead of the conventional direct sequence. These new methods permit energy savings more than 30% in comparison with conventional sequence distillation columns.

Moreover, the recent rise in energy prices and demands further emphasizes the relevance of this problem.

## 1. Introduction

Distillation is a physical process for the separation of liquid mixtures that is based on differences in the boiling points of the constituent components. Distillation is the most widely separation process used in many industries.

### 1.1. Distillation applications

Distillation makes about 95% of all current industrial separation processes. It has been used in chemical industries, pharmaceutical and food industries, environmental technologies and in petroleum-refineries.

The most common use is after a chemical reactor where we obtain some products. Distillation is used in order to separate the desired product from the rest obtaining a high purity product.

Examples of the most important applications in food industries are concentrating essential oils and flavors; the deodorization of fats and oils or in alcohol distillation. Some pharmaceutical processes based on concentration of antibiotics are also related with distillation columns.

On the other hand, distillation is the main part in petroleum refineries. The crude oil which contains a complex mixture of hydrocarbons is pumped into a huge distillation column in order to be separated them by different temperatures.

Environmental legislation is becoming very strict. Consequently, plants for the recovery and cleaning of solvents are continually gaining in importance in order to avoid the waste emit into the environment. So separation processes are very important, and distillation is one of this which is used for example in water treatments, etc...

As we can see, distillation is applied for many different processes because of its reliability, simplicity and low-capital costs although these systems have relatively high energy consumption. However, there are many active researches regarding making the process more energy efficient, which will be discussed in more detail later in the text.

### 1.2 Distillation theory

The process of distillation begins with a feed stream that requires treatment. The feed is separated into two fractions in a conventional column (Fig1.): the light product and the heavy product. Throughout the report, the feed molar flow rate  $F$  will be reported by (kgmole/h) feed mole fraction is  $z$  and the stage that feed enters is denoted by  $N_F$  (normally the tray on which the characteristics of the fluid is closest to that of the feed)

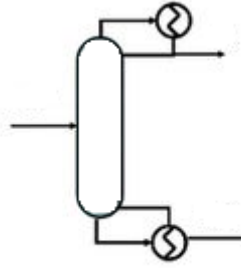


Fig1. Distillation Column

As it shown in Fig.1 the liquid leaving the top of the column is the light component, while the liquid leaving the bottom of the column is the heavy component. Liquid leaving the bottom of the column is split into a bottoms product and a fraction that is made available for boiling. The reboiler (heat exchanger) is employed to boil the portion of the bottom liquid that is not drawn off as product. The vapor produced flows up through the column and comes into intimate contact with the downflowing liquid. After the vapor reaches and leaves the top of the column, another heat exchanger (the condenser) is encountered where heat is removed from the vapor to condensate it. The condensed liquid is split into two streams. One is the overhead product; the other liquid stream is called reflux and is returned to the top of the column to improve the separation.

### 1.2.1 Fundamental concepts

The vapour-liquid equilibrium on each stage is the central part of the distillation theory. The most difficult part in the distillation column design is the description of this equilibrium between the vapour and the liquid.

To derive the following equations, we base on ideal mixtures so the vapour-liquid equilibrium can be derived from Raoult's law: The partial vapour pressure of a component in a mixture is equal to the vapour pressure of the pure component at the temperature multiplied by its mole fraction in the mixture.

$$p_i = x_i p_i^0(T)$$

For an ideal gas, according to Dalton's law:

$$p_i = y_i P$$

Therefore, the equilibrium between the vapour and the liquid for ideal mixtures is:

$$y_i = x_i \frac{p_i}{P}$$

**Note:** However we have assumed ideal equilibrium vapour-liquid, actually there are few systems that work as ideal mixtures. For this reason, the simulations will be done with non-ideal mixtures.

### 1.2.2. Column design

Taking the column in Fig. 1 into consideration, the following material balances can be applied to the external and internal flows. For the first ones the total flow balance is:

$$F = D + B$$

And for a component balance:

$$F \cdot z = D \cdot x_D + B \cdot x_B$$

Once all the balances are developed, McCabe-Thiele method is the most widely way to find the number of equilibrium stages for a given feed.

It is started by plotting the vapour-liquid equilibrium. The next step is to define the feed line. The condition of the feed determines the difference in vapour and liquid flow rates between the rectifying section (section above the feed stage) and the stripping section (bottom section).

The last step is to plot the rectifying operating line and the stripping operating line with the following equations:

$$y_n = \left(\frac{L}{V}\right)_T (x_{n+1} - x_D) + x_D \quad \text{Rectifying line}$$

$$y_n = \left(\frac{L}{V}\right)_B (x_{n+1} - x_B) + x_B \quad \text{Stripping line}$$

Then a typical McCabe-Thiele diagram can be plotted:

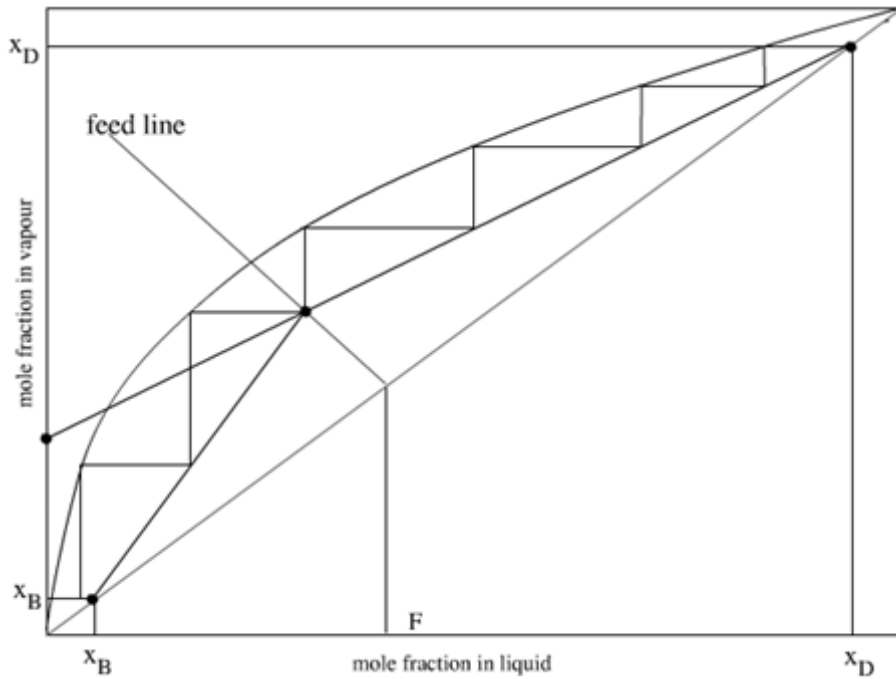


Fig2. McCabe-Thiele Diagram.

Using McCabe-Thiele method, the two limiting cases can be determined:

Total Reflux (minimum ideal stages)

The total reflux condition represents operation with no product removal. The entire overhead vapor is condensed and returned as reflux. Consequently, the reflux ratio (L/D) is infinite. This, in turn, makes the operating lines the 45 degree. Thus, the distance between the equilibrium curve and the operating lines is large, so the stepping triangles become bigger, so there will be fewer stages.

For a column with N stages, the separation factor is described by:

$$S = \frac{\left(\frac{x_L}{x_H}\right)_T}{\left(\frac{x_L}{x_H}\right)_B} = \alpha^N$$

For a column with a given separation, the minimum number of stages is:

$$N_{min} = \frac{\ln S}{\ln \alpha}$$

A rule of thumb to select the actual number of stages is based on the minimum number of stages, and it is usually twice the minimum.

### Minimum Reflux (infinite ideal stages)

In this case, the intersection of the operating lines lies on the equilibrium curve itself. Thus, the distance between the equilibrium curve and the operating lines is at its minimum, the stepping triangles become very small.

At minimum reflux, the mixing is less important than in minimum ideal stages. For this reason a pinch zone, which is a zone of constant composition, will develop. This means that there will be zones that there will not change in the composition from stage to stage.

### 1.3. Different types of columns

In the former section, we talked about a conventional column which contains one reboiler and one condenser. The thermal energy added at the reboiler is used to evaporate a liquid mixture and is lost when liquefying the vapor flow at the condenser to obtain the reflux. However, the thermal energy recovered at the condenser cannot be used to heat other flows in the same distillation column since the temperature of the cooling medium is usually lower than the flows inside the column. The other problem is the inefficiency due to the remixing happens in the conventional columns, for example when the reflux is fed to the column.

To improve the low energy efficiency of conventional columns and because of the drastic increase in energy cost, new saving-configurations have become attractive. These include the thermally coupled distillation systems and internally heat-integrated distillation column (HIDiC)

#### 1.3.1 Thermally coupled distillation

Thermally coupled distillation column is an example of the new configurations studied. It requires only one condenser or one reboiler. This results in low energy input and high thermal efficiency. Thermally coupled distillation columns are those that are linked together by their overhead and bottom streams without heat exchangers.

The most important thermally coupled distillation sequence is Petlyuk column (Fig.3) This Petlyuk configuration for a 3 component separation consists of two interconnected columns. The first column, called prefractionator, performs a non-sharp separation for the middle component. In the second column the mixture of the lightest and the middle component is separated in the upper part of the column, while in the bottom the middle and the heaviest component are separated. The two columns are linked by recycle flows from the main column into the top and the bottom of it.

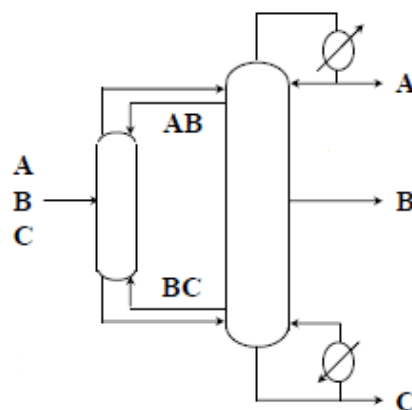


Fig3. Petlyuk distillation column.

Other thermally coupled configuration is the DWC, divided wall column or Kaibel column (Fig4.) It consists of a single shell column with a partitioning wall that separates the feed location from the side draw of the middle component. The liquid reflux from the condenser and the vapour from the reboiler are splitted into two parts for the two sides of the wall (prefractionator and main column).

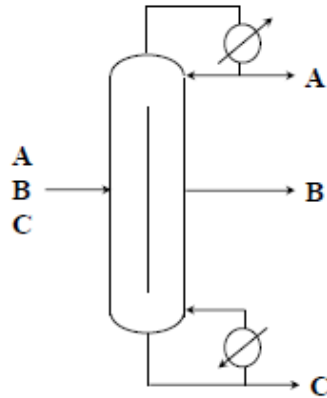


Fig4. Kaibel column

The Petlyuk and the DWC configurations can be considered equivalent from the energetic point of view assuming that no heat transfer across the wall occurs.

### 1.3.2.HIDiC

In the conventional distillation column, the temperature of the rectifying section is lower than that of the stripping section. If the former is higher than the latter, the residual heat of the rectifying section can be used in the stripping section. To realize this, the pressure of the rectifying section must be sufficiently high, so that the vapor coming from the stripping section is compressed.

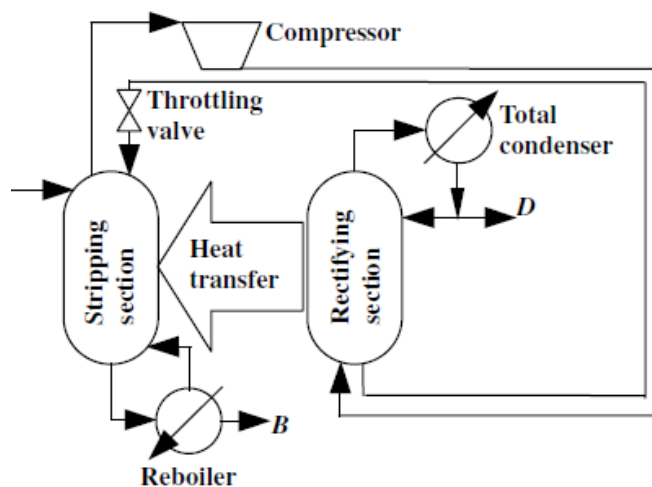


Fig5. Schematic diagram of a HIDiC [2]



Therefore, HIDic column is a tray column consisting of a reboiler and total condenser. In addition, HIDic has a compressor and a throttling valve, and the rectifying and stripping section are heat-coupled to each other. In the figure (Fig5.) we can see a schematic diagram of this new configuration.

## 2. Minimum energy requirements

With a given feed and constant pressure a binary distillation column has only two degrees of freedom (because of the reboiler and the condenser) For multicomponent feed, one usually specifies the distribution of two key components and then the distribution of the non-key components is completely determined for a given feed.

### 2.1. Underwood's Method

The Underwood method will provide a quick estimate of minimum reflux requirements. Starting with the net material transport in the stage  $n$ , as the difference between the amount travelling upwards (which is defined positive) as vapour and the amount entering a stage as liquid:

$$w_i = V_n \cdot y_{i,n} - L_{n+1} \cdot x_{i,n+1}$$

To derive the corresponding equations, constant molar flow and constant relative volatility have been assumed.

The vapour-liquid equilibrium in the former equation:

$$y_i = \frac{\alpha_i \cdot x_i}{\sum_i \alpha_i \cdot x_i}$$

With these two equations, we can obtain the definition equation as:

$$V = \sum_{i=1}^N \frac{\alpha_i \cdot w_i}{\alpha_i - \phi}$$

#### 2.1.1. Definition of Underwood roots

The definition equation can be used for the top section and bottom section.

Underwood roots in the top section ( $\phi$ ) are defined as:

$$V_T = \sum_{i=1}^N \frac{\alpha_i \cdot w_{i,T}}{\alpha_i - \phi}$$

Where  $w_{i,T}$  is defined as

$$w_{i,T} = D \cdot x_{i,D} = r_{i,D} \cdot z_i \cdot F$$

In the same way, defining the Underwood roots ( $\Psi$ ) in the bottom section:

$$V_B = \sum_{i=1}^N \frac{\alpha_i \cdot w_{i,B}}{\alpha_i - \Psi}$$

Where  $w_{i,B}$  is defined as

$$w_{i,B} = -B \cdot x_{i,B} = -r_{i,B} \cdot z_i \cdot F$$

Finally, recalling the relationship between the vapour flows as:

$$V_T - V_B = (1 - q)F$$

Then,

$$\sum_{i=1}^N \frac{\alpha_i \cdot w_{i,T}}{\alpha_i - \phi} - \sum_{i=1}^N \frac{\alpha_i \cdot w_{i,B}}{\alpha_i - \Psi} = (1 - q)F$$

Before we discussed that the components flow upwards in the top section are defined positive, so  $w_{i,T} \geq 0$  and downwards in the top section  $w_{i,B} \leq 0$ . This means that there are  $N_c$  solutions for  $N_c$  components.

$$\alpha_i - \phi_i > 0$$

$$\alpha_i - \Psi_i < 0$$

When the vapour flow is reduced, the roots in the top section will decrease, while the roots in the bottom section will increase. Then the minimum reflux (minimum energy that implies minimum vapor flow) occurs when:

$$\phi_i = \Psi_{i+1} = \theta_i$$

In the next figure, it is shown the top and bottom approach to the common roots.

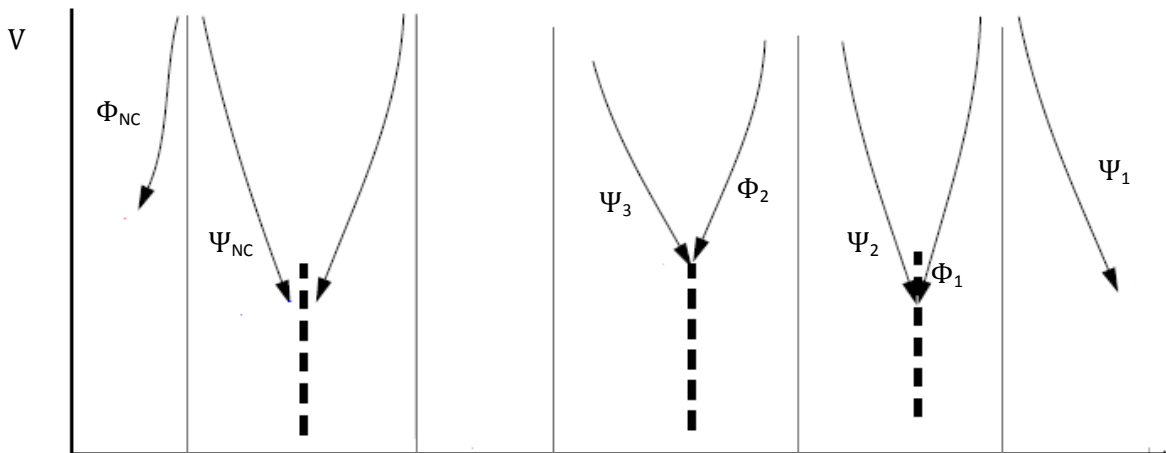


Fig6. Common Roots, Underwood equations.

Finally, we can obtain the following equation (feed equation) for the common roots  $\theta$ :

$$(1 - q) = \sum_{i=1}^N \frac{\alpha_i \cdot z_i}{\alpha_i - \theta}$$

With this equation, the common roots can be calculated without knowing anything about the distribution of feed components in the products.

Replacing the active root in the top and bottom definition equation gives the minimum flow:

$$V_{Tmin} = \sum_{i=1}^N \frac{\alpha_i \cdot w_{i,T}}{\alpha_i - \theta}$$

### 2.1.2. Computation procedure

The objective is to find the product recoveries and the vapour flow. The two main equations are the feed equation which gives us the possible common roots, and the definition equations (in the top or in the bottom) which give us the actual roots for a given flow and product distribution.

First of all, the common roots should be computed. There are  $N_C - 1$  common roots which obey:

$$\alpha_1 > \theta_1 > \alpha_2 > \theta_2 > \dots > \theta_{N_C-1} > \alpha_{N_C}$$

Once they are obtained from the feed equation the next step is to compute the minimum energy for a sharp split between two adjacent components using the definition equation:

$$V_{Tmin} = \sum_{i=1}^N \frac{\alpha_i \cdot w_{i,T}}{\alpha_i - \theta}$$

Finally we have to consider the sharp split between the most heavy and most light components, while intermediates are distributed to both products. In this case, we have to solve a linear equation set which the unknown variables are the recoveries for the distributed components and the vapour flow:

$$V_{Tmin} = \sum_{i=1}^N \frac{\alpha_i \cdot r_{i,T} \cdot z_i}{\alpha_i - \theta_1}$$

$$V_{Tmin} = \sum_{i=1}^N \frac{\alpha_i \cdot r_{i,T} \cdot z_i}{\alpha_i - \theta_2}$$

...

$$V_{Tmin} = \sum_{i=1}^N \frac{\alpha_i \cdot r_{i,T} \cdot z_i}{\alpha_i - \theta_{Nc-1}}$$

Where we only know that  $r_{1,T}$  is equal to 1 and  $r_{Nc,T}$  is equal to 0.

## 2.2. The V-min diagram

As we discussed above, with a given feed and constant pressure a binary distillation column has only two degrees of freedom so the operating points can be visualized in two dimensions. These two dimensions chosen are the top vapor flow ( $V_T$ ) and the product split ( $D$ )

The diagram provides an informative visualization for any set of specifications and infinite number of stages for a 3-component feed.

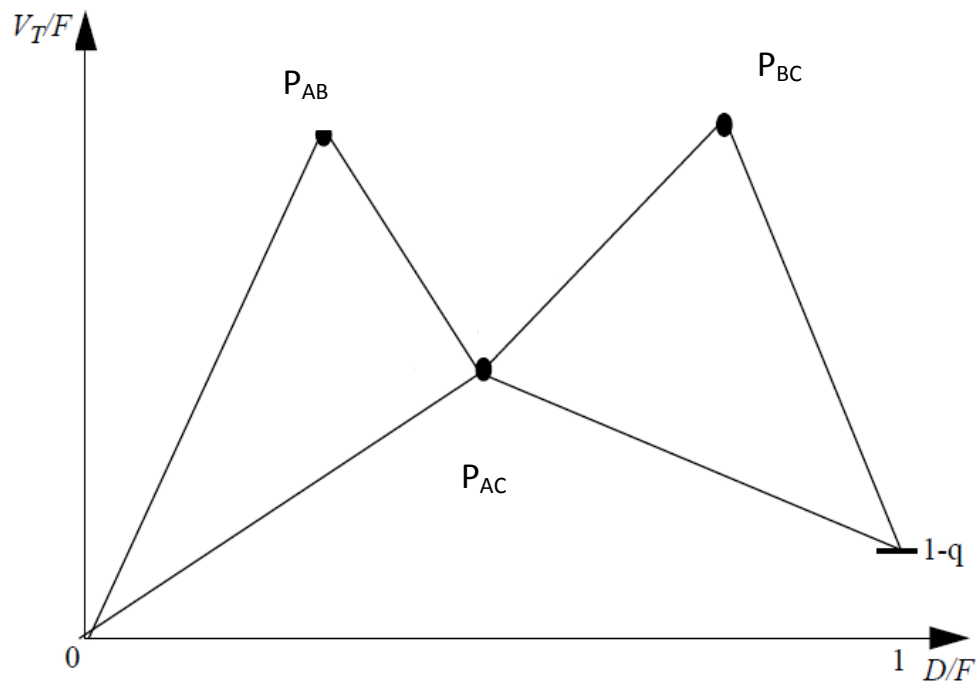


Fig7. The Vmin-diagram for a ternary mixture ABC

### 2.2.1. Procedure for Multicomponent case

The procedure to draw the above Vmin-diagram is as follows:

1. Find the common roots from the feed equation
2. Find the peaks and knots and the “preferred split”:
  - 2.1. Compute  $N_C - 1$  peaks. We can calculate the minimum energy applying the definition equation for the top.

$$V_T = \sum_{i=1}^N \frac{\alpha_i \cdot w_{i,T}}{\alpha_i - \phi}$$

The recoveries will be:

$$r_{i,D} = 1 \text{ for } i \leq j$$

$$r_{i,D} = 0 \text{ for } i \geq j$$

- 2.2. Compute  $N_C - 2$  knots (cases with one distributed component) In that case set  $r_{1,D} = 0$  and  $r_{N_C,D} = 0$  and solve linear equation set, in each knot we have to calculate the respective recovery for the distributed component.
  - 2.3. Compute the “preferred split” solution where the all intermediates are distributed. In this case, we have to calculate a linear equation set, where we have as unknown variables the recoveries of the distributed components and the vapour flow.
3. Find the asymptotic points where all recoveries in the top are zero and one, respectively.

$$(V_{Tmin}, D) = (0, 0)$$

$$(V_{Tmin}, D) = (1-q, 1)$$

### 2.3. Sample case for a four component feed

Consider the separation of a mixture of four alcohols. In the following table feed composition and relative volatilities are included:

Table1. Data for the example

Components	Feed composition	Relative volatility
Methanol	0.25	7.6
Ethanol	0.25	4.6
n-propanol	0.25	2.24
n-butanol	0.25	1

F=100 kgmole/h

q, liquid fraction=1

Note: The specification of composition fraction impurity will be 1%

#### 2.3.1. Underwood equations procedure

We follow the computation procedure for the 4-component case:

1. Find all the possible common roots from the feed equation.

With four components, there are 3 common roots, so first of all we have to solve all of them.

$$\frac{\alpha_A z_A}{\alpha_A - \theta_A} + \frac{\alpha_B z_B}{\alpha_B - \theta_A} + \frac{\alpha_C z_C}{\alpha_C - \theta_A} + \frac{\alpha_D z_D}{\alpha_D - \theta_A} = 0$$

$$\frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{\alpha_B z_B}{\alpha_B - \theta_B} + \frac{\alpha_C z_C}{\alpha_C - \theta_B} + \frac{\alpha_D z_D}{\alpha_D - \theta_B} = 0$$

$$\frac{\alpha_A z_A}{\alpha_A - \theta_C} + \frac{\alpha_B z_B}{\alpha_B - \theta_C} + \frac{\alpha_C z_C}{\alpha_C - \theta_C} + \frac{\alpha_D z_D}{\alpha_D - \theta_C} = 0$$

Solving these three equations, we can obtain the 3 common roots, so:

$$\theta_A = 5.92$$

$$\theta_B = 2.86$$

$$\theta_C = 1.21$$

2. Determine the total set of the distributed components Nd

In the four components feed, we have two distributed components. This means, as we saw above, that the components in the feed appear in both products. B and C are the both distributed components.

There will be  $N_d - 1$  active Underwood roots that correspond with these distributed components.

3. Apply the set of definition equations corresponding to each active root.

Peaks

The peaks represent sharp splits, no distributing components:

$P_{AB}$ :

$$[r_{A,T}, r_{B,T}] = [1, 0]$$

$$[D/F, V_{Tmin}] = [z_A, \frac{\alpha_A z_A}{\alpha_A - \theta_A}] = [0.25, 1.088]$$

$P_{BC}$ :

$$[r_{B,T}, r_{C,T}] = [1, 0]$$

$$[D/F, V_{Tmin}] = [z_A + z_B, \frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{\alpha_B z_B}{\alpha_B - \theta_B}] = [0.5, 1.059]$$

$P_{CD}$ :

$$[r_{C,T}, r_{D,T}] = [1, 0]$$

$$[D/F, V_{Tmin}] = [z_A + z_B + z_C, \frac{\alpha_A z_A}{\alpha_A - \theta_C} + \frac{\alpha_B z_B}{\alpha_B - \theta_C} + \frac{\alpha_C z_C}{\alpha_C - \theta_C}] = [0.75, 1.178]$$

Knots

The knots represent the case when one of the products is distributed.

$P_{AC}$ :

$$[r_{A,T}, r_{C,T}] = [1, 0]$$

In this case, we have two unknown variables: the recovery of B  $r_{B,T}$  and the vapour flow. Therefore, to solve this problem, we need two equations:

$$V_{Tmin} = \frac{\alpha_A z_A}{\alpha_A - \theta_A} + \frac{r_{B,T} \alpha_B z_B}{\alpha_B - \theta_A}$$

$$V_{Tmin} = \frac{\alpha_A z_A}{\alpha_A - \theta_A} + \frac{r_{B,T} \alpha_B z_B}{\alpha_B - \theta_B}$$

With these two equations, we obtain:

$$V_{Tmin} = 0.693$$

$$r_{B,T} = 0.438$$



With the recovery of B, we can calculate D:

$$\frac{D}{F} = z_A + r_{B,T}z_B = 0.362$$

P<sub>BD</sub>:

$$[r_{B,T}, r_{C,T}] = [1, r_{C,T}]$$

As above, we have two unknown variables: the recovery of C  $r_{C,T}$  and the vapour flow. Therefore, to solve this problem, we need two equations:

$$V_{Tmin} = \frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{\alpha_B z_B}{\alpha_B - \theta_B} + \frac{r_{C,T} \alpha_C z_C}{\alpha_C - \theta_B}$$

$$V_{Tmin} = \frac{\alpha_A z_A}{\alpha_A - \theta_C} + \frac{\alpha_B z_B}{\alpha_B - \theta_C} + \frac{r_{C,T} \alpha_C z_C}{\alpha_C - \theta_C}$$

With these two equations, we obtain:

$$V_{Tmin} = 0.792$$

$$r_{C,T} = 0.28$$

With the recovery of B, we can calculate D:

$$\frac{D}{F} = z_A + z_B + r_{C,T}z_C = 0.572$$

Preferred split

The preferred split represents the case when all the intermediates are distributed to both products.

P<sub>AD</sub>:

$$[r_{A,T}, r_{B,T}, r_{C,T}] = [1, r_{B,T}, r_{C,T}]$$

In this case, we have three unknown variables: the recovery of B  $r_{B,T}$ , the recovery of C  $r_{C,T}$  and the vapour flow. Therefore, to solve this problem, we need three equations:

$$V_{Tmin} = \frac{\alpha_A z_A}{\alpha_A - \theta_A} + \frac{r_{B,T} \alpha_B z_B}{\alpha_B - \theta_A} + \frac{r_{C,T} \alpha_C z_C}{\alpha_C - \theta_A}$$

$$V_{Tmin} = \frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{r_{B,T} \alpha_B z_B}{\alpha_B - \theta_B} + \frac{r_{C,T} \alpha_C z_C}{\alpha_C - \theta_B}$$

$$V_{Tmin} = \frac{\alpha_A z_A}{\alpha_A - \theta_C} + \frac{r_{B,T} \alpha_B z_B}{\alpha_B - \theta_C} + \frac{r_{C,T} \alpha_C z_C}{\alpha_C - \theta_C}$$

With these two equations, we obtain:

$$V_{Tmin} = 0.582$$

$$r_{B,T} = 0.541$$

$$r_{C,T} = 0.189$$

With the recovery of B and C, we can calculate D:

$$\frac{D}{F} = z_A + r_{B,T} z_B + r_{C,T} z_C = 0.432$$

Table2. Operating point for example of 4-components with underwood equations

<b>Operating Point</b>	<b>P<sub>AB</sub></b>	<b>P<sub>BC</sub></b>	<b>P<sub>CD</sub></b>	<b>P<sub>AC</sub></b>	<b>P<sub>BD</sub></b>	<b>P<sub>AD</sub></b>
<b>D/F</b>	0.25	0.5	0.75	0.362	0.572	0.432
<b>V<sub>T</sub>/F</b>	1.088	1.059	1.178	0.693	0.792	0.582

### 2.3.2. Unisim procedure

Unisim is a powerful computer tool that helps engineers simulate the processes.

The first step in Unisim is to create the case with the components and the most suitable fluid package. Also, we need to set the number of stages, the pressure in the column and two other specifications. As a distillation column has two degrees of freedom, to converge the problem we need two specifications which are usually chosen as the impurities of light and heavy component in the bottom and the top respectively.

As we discussed before, the minimum energy is obtained working with an infinite number of trays. So in this case, we assume 100 trays, that means working like this. In the next table the results are presented.

Table3. Operating point for example of 4-components with Unisim

Operating Point	$P_{AB}$	$P_{BC}$	$P_{CD}$	$P_{AC}$	$P_{BD}$	$P_{AD}$
<b>D</b>	24.49	50	75.51	36.03	57.87	43.35
<b>V<sub>T</sub></b>	110.9	107.8	119.7	70.18	79.51	57.87

In the Fig8. V-min diagram is plotted from the Underwood equations and also from Unisim results.

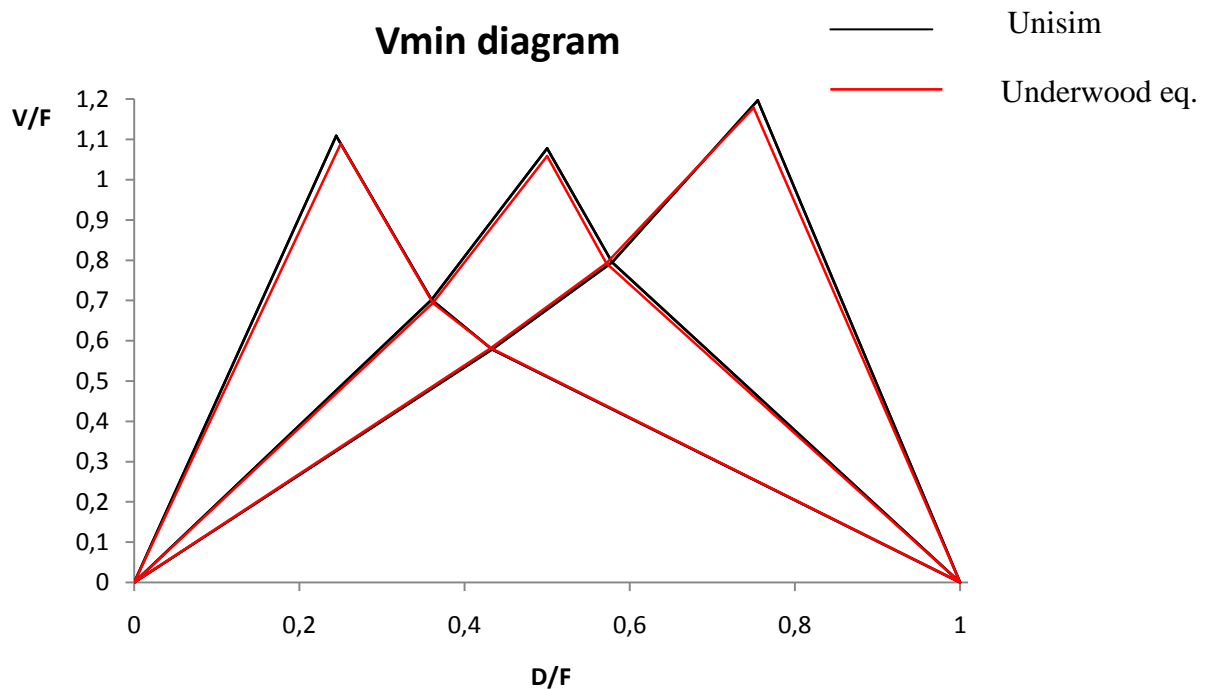


Fig8. V-min diagram for 4 components example.

Comparing both Vmin diagrams, we can see that for Underwood equations, we obtain the minimum for the two. This is because for the Underwood equations we assume infinite number of trays; whereas in Unisim we cannot work with this assumption (we choose 100 in order to try to simulate this situation)

The V-min diagram gives a simple graphical interpretation of the whole operating space. The distribution of feed components and corresponding minimum energy requirement is easily in the diagram. The characteristic peaks and knots represent minimum energy operation for sharp split between all possible pairs of key components.

## 2.4. Underwood equations applied to thermally coupled sections

Before starting with more difficult configurations, some remarks about the thermally coupled columns should be discussed.

As we saw above, the thermally coupled columns have recycle flows (vapour flow entering at the bottom and liquid flow entering at the top) This is a new situation compared to the conventional arrangements, so we must check how the recycle streams affect the split of components. The next rule has been deduced to ask the question above: A component which would have been removed does not appear in the side stream of the first column. For instance, if A/D split is considered, the heaviest component cannot appear in the top of the column, so the side stream cannot contain this component.

To consider this question, we simulate the prefractionator in Unisim. We use the optimizer to remain the value of D constant when the side streams change. D is defined as the difference between  $V_T$  and  $L_T$  as we can see in Fig9:

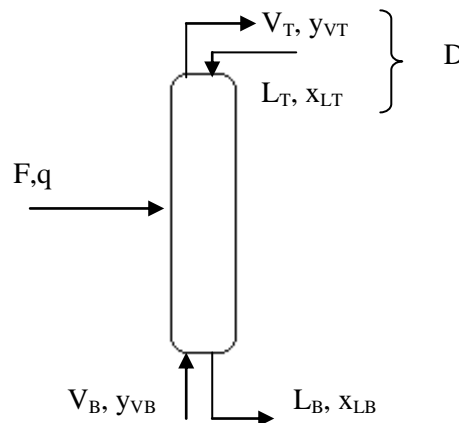


Fig9. The prefractionator of a Petlyuk arrangement.

In this case we change the composition of the liquid lateral stream entering at the top, and we use the recoveries to see if they remain constant with different compositions. Defining the recoveries as:

$$r_{i,T} = \frac{w_{i,T}}{w_{i,F}}$$

Where the net component flow in the feed,  $w_{i,F}$ , is defined as the product between the composition and the net flow in the feed, whereas as we saw before, the net component flow in the top,  $w_{i,T}$ , is defined as the product between the composition and the net flow in the top.

Table 4.Recoveries for different compositions

<b>Components</b>	<b>Feed composition</b>	<b>Recoveries</b>	<b>Feed Composition</b>	<b>Recoveries</b>
Methanol	0.65	0.517121	0.7	0.517121
Ethanol	0.35	0.53264	0.3	0.532638
n-propanol	0	0.65332	0	0.653319
n-butanol	0	0.066752	0	0.066754

Another comment about the thermally coupled is the benefit of using it. In the conventional column remixing occurs caused by recycling of the condenser and reboiler products, so in the ends of the column the composition drops because of remixing. Instead, in the thermally coupled columns there is no remixing, so the composition does not change from stage to stage.

### 3. Distillation sequences

#### 3.1. Introduction

As it is introduced before, a simple distillation column separates a feed mixture into two products. If the feed mixture consists of more than two components and more than two products are required, then the continuous separation is accomplished by multiple distillation columns in series. Several possibilities may be discussed, such as direct sequences, columns in series where the most volatile product is removed first column; an indirect sequence, columns in series where the least volatile component is removed first.

The separation of a multi-component mixture is conventionally accomplished in a series of columns, each having a condenser and a reboiler. These conventional distillation columns require, as we discussed above, high energy input.

Thermally coupled distillation columns can be used for multi-component separations in order to reduce the energy consumption.

With this part of the report, it will be shown that distillation systems (thermally coupled configurations) with less than N-1 columns have the potential to save both energy and capital costs compared to the conventional simple column configurations where N-1 are employed.

#### 3.2. Case four components feed

The study will be for the 4- component separation studied above.

##### 3.2.1. Simple column configurations

The procedure to develop all distillation sequences for simple columns starts by drawing all the possible configurations. It is known that for an N-component separation the number of simple column sequences ( $S_n$ ) can be predicted with:

$$S_n = \frac{[2(N - 1)]!}{N! (N - 1)!}$$

For a four-component mixture, then, there will be 5 possible simple columns configuration, as it is presented in Fig. 10:

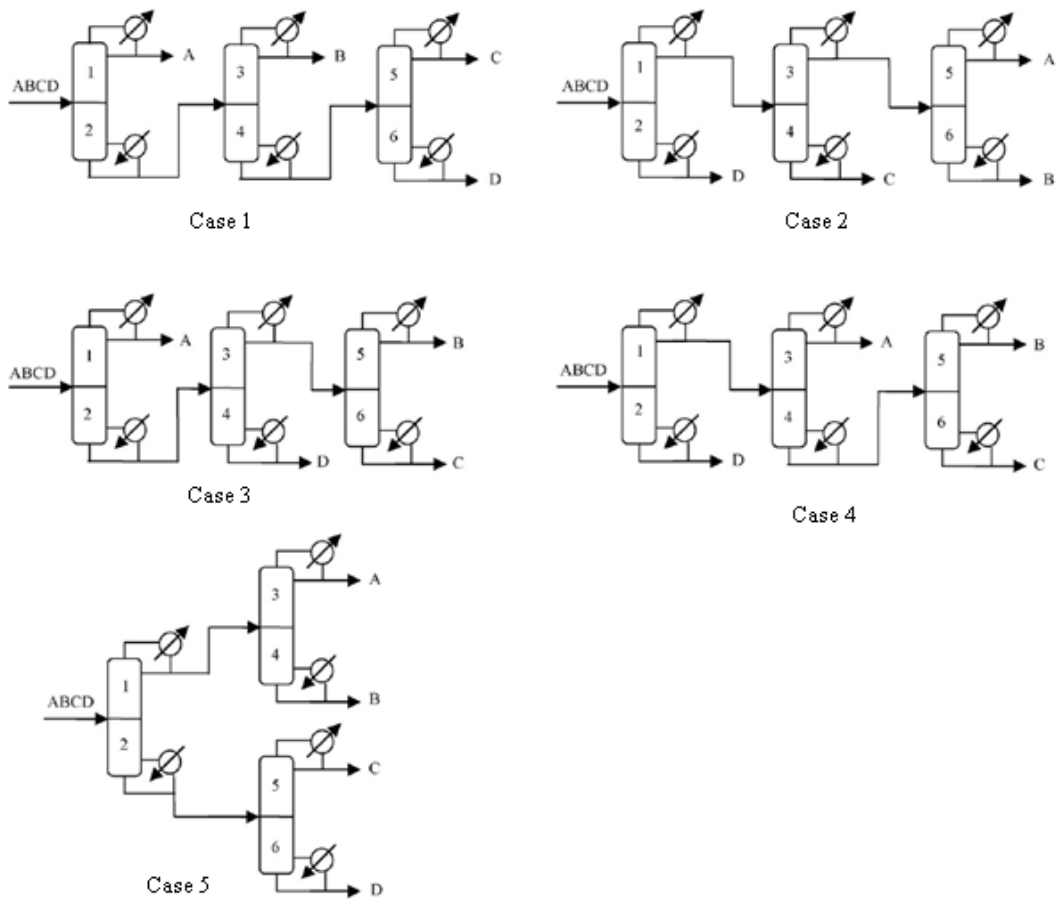


Fig10. Simple column configuration for a four-component mixture [5]

The energy requirements for the condenser and the reboiler for a sharp split in each column will be obtained with an infinite number of stages  $N=100$  (as it has been explained before corresponded with the minimum energy) and with a realistic number of stages, 25 and then we will be able to compare the energy consumptions for these two cases:

Table5. Energy requirements for different simple column configurations (N=100)

	<b>Case 1</b>			<b>Case 2</b>		
<b>Energy condenser (kW)</b>	Col1. 1088	Col2. 861	Col3. 805.6	Col1. 1314	Col2. 1066	Col3. 971.7
<b>Energy reboiler (kW)</b>	1131	866.3	794.2	1335	1103	991.1
	<b>Case 3</b>			<b>Case 4</b>		
<b>Energy condenser (kW)</b>	Col1. 1088	Col2. 1083	Col3. 775.8	Col1. 1276	Col2. 1045	Col3. 761.5
<b>Energy reboiler (kW)</b>	1131	1066	806.7	1308	1071	769.5
	<b>Case 5</b>					
<b>Energy condenser (kW)</b>	Col1. 1113	Col2. 967.5	Col3. 800.4			
<b>Energy reboiler (kW)</b>	1157	968.7	789.1			

Table6. Energy requirements for different simple column configurations (N=25)

	<b>Case 1</b>			<b>Case 2</b>		
<b>Energy condenser (kW)</b>	Col1. 1552	Col2. 1002	Col3. 930	Col1. 1352	Col2. 1160	Col3. 1684
<b>Energy reboiler (kW)</b>	1594	1008	918.6	1373	1197	1704
	<b>Case 3</b>			<b>Case 4</b>		
<b>Energy condenser (kW)</b>	Col1. 1552	Col2. 1145	Col3. 922.6	Col1. 1303	Col2. 1710	Col3. 904.8
<b>Energy reboiler (kW)</b>	1594	1128	953.5	1336	1736	912.8
	<b>Case 5</b>					
<b>Energy condenser (kW)</b>	Col1. 1206	Col2. 1675	Col3. 924.1			
<b>Energy reboiler (kW)</b>	1251	1695	912.8			

The next step is to compare the costs of the distillation column equipment and the costs of energy consumption.

To compute the cost of distillation column equipment, the sum of the costs of column shell and trays should be considered.

Column shell:

$$\$ = \left( \frac{M\&S}{280} \right) (937.61) D^{1.066} H^{0.802}$$



$$H = (N - 1) \cdot 0.6 + 6.0 \quad (1)$$

Column trays:

$$\$ = \left( \frac{M\&S}{280} \right) (97.24) D^{1.55} h$$

Where:

D: the diameter of the column (m) Its value is 1.5 m

H: the height of the column. It can be calculated with the equation (1) where N is the number of trays

M&S: Marshall and Swift cost index which can be found in [6]

H: the tray stack height (m)

Using these two correlations we can know the cost estimation of the process, the next table presents the results:

Table7. Cost estimations for different simple column configurations

Cost estimations	Case N=100	Case N=25
Cost Column Shell (\$)	198,966.22	78,164.47
Cost Column trays(\$)	48,316.96	7,247.54
Total cost (\$)	247,283	85,412

On the other hand, the heat exchanger cost evaluation is based on the heat exchanger area:

$$\$ = \left( \frac{M\&S}{280} \right) (474.67) A^{0.65}$$

The heat exchanger area is evaluated using the usual design formula:

$$A = \frac{Q_{c/r}}{U_d \Delta T_{LM}}$$

Where:

$Q_{c/r}$ : Condenser duty and reboiler duty respectively (kW)

$U_d$ : heat transfer coefficient ( $\text{kJ m}^{-2} \text{h}^{-1} \text{°C}^{-1}$ )

$\Delta T_{LM}$ : logarithmic mean temperature difference

In distillation columns, Unisim calculates the duty of condensers and reboilers, but not the heat exchanger area for the capital cost estimation. So, to estimate the heat exchanger area, we have simulated condensers and reboilers using the heat exchanger unit in Unisim. Searching in the literature, an average value for the heat transfer coefficient has considered, 150 Btu/F ft<sup>2</sup> h [8]. The results are presented in the next table:

Table8. Heat exchangers cost evaluation N=100

	Heat exchanger	UA	A,m <sup>2</sup>	Cap. Cost \$
<b>Case 1</b>	Con1.	170000	53.64	30445
	Con2.	82400	26	19014
	Con3.	49700	15.68	13688
	Reb1.	73445	23.17	17644
	Reb2.	75844	23.93	18017
	Reb3.	106610	33.64	22480
	Total			121288
<b>Case2</b>	Con1.	119000	37.49	24902
	Con2.	125000	39.38	27054
	Con3.	142000	44.73	31448
	Reb1.	178996	56.38	18979
	Reb2.	82307	25.93	14188
	Reb3.	52609	16.57	76300
	Total		220.47	192871
<b>Case3</b>	Con1.	170000	53.55	19469
	Con2.	85600	26.96	17571
	Con3.	73100	23.03	17637
	Reb1.	73525	23.16	27269
	Reb2.	143739	45.28	15476
	Reb3.	60129	18.94	69486
	Total		190.92	166907
<b>Case 4</b>	Con1.	123000	38.75	31448
	Con2.	179000	56.39	17099
	Con3.	70100	22.08	23727
	Reb1.	116045	36.55	14432
	Reb2.	54004	17.01	13476
	Reb3.	48601	15.31	68337
	Total		186.09	168519
<b>Case 5</b>	Con1.	131000	41.27	28035
	Con2.	150000	47.25	13976
	Con3.	51400	16.19	21691
	Reb1.	101081	31.84	14139
	Reb2.	52330	16.48	22399
	Reb3.	106199	33.45	68432
	Total		186.48	168672

Table9. Heat exchangers cost evaluation N=25

	Heat exchanger	UA	A,m <sup>2</sup>	Cap. Cost, \$
<b>Case1</b>	Con1.	242000	76.23	21259
	Con2.	98000	30.87	15421
	Con3.	59800	18.83	22800
	Reb1.	109138	34.38	24640
	Reb2.	122981	38.74	20074
	Reb3.	89726	28.26	77831
	Total			227.32
<b>Case2</b>	Con1.	123000	38.75	26305
	Con2.	136000	42.84	40285
	Con3.	262000	82.53	32126
	Reb1.	184970	58.27	10032
	Reb2.	30866	9.72	20191
	Reb3.	90532	28,52	85064
	Total			260,62
<b>Case3</b>	Con1.	242000	76.23	20230
	Con2.	90800	28.6	20143
	Con3.	90200	28.41	21937
	Reb1.	102849	32.4	28285
	Reb2.	152059	47.9	17269
	Reb3.	71178	22.42	79742
	Total			235.96
<b>Case 4</b>	Con1.	125000	39.38	43226
	Con2.	292000	9,98	19128
	Con3.	83300	26.24	24055
	Reb1.	118515	37.33	19717
	Reb2.	87282	27.49	15073
	Reb3.	57737	18.19	80759
	Total			240,61
<b>Case 5</b>	Con1.	142000	44.73	40185
	Con2.	261000	82.22	15353
	Con3.	59400	18.71	22800
	Reb1.	109138	34.38	20074
	Reb2.	89726	28.26	24640
	Reb3.	122981	38.74	82156
	Total			247.04

### 3.2.2. Thermally coupled configurations

The total number of thermally coupled schemes can be calculated from the following formula:

$$P_n = \frac{[2(N-1)]!}{N!(n-1)!} \left[ \sum_{j=1}^{N-3} \frac{(N-2)!}{j!(N-2-j)!} + 1 \right]$$

Each thermally coupled configuration can be obtained from the corresponding simple column sequence by substituting one or more condenser/s and/or reboiler/s associated to no product streams with a bidirectional vapour-liquid connection. Fig.12 presents all of the thermally coupled configurations considered as an alternative for the 4-components separation:

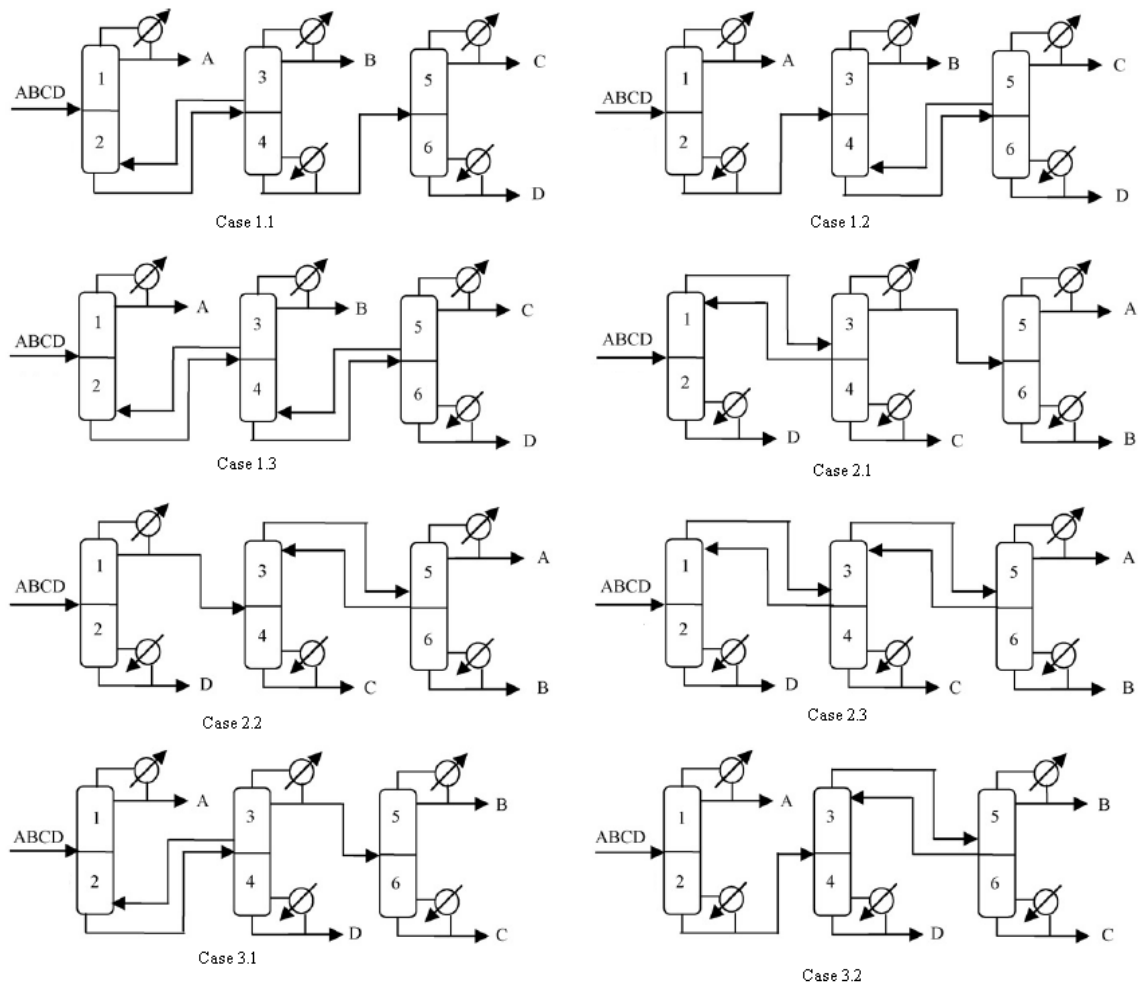


Fig 11. Thermally coupled distillation configurations for a four-components [5]

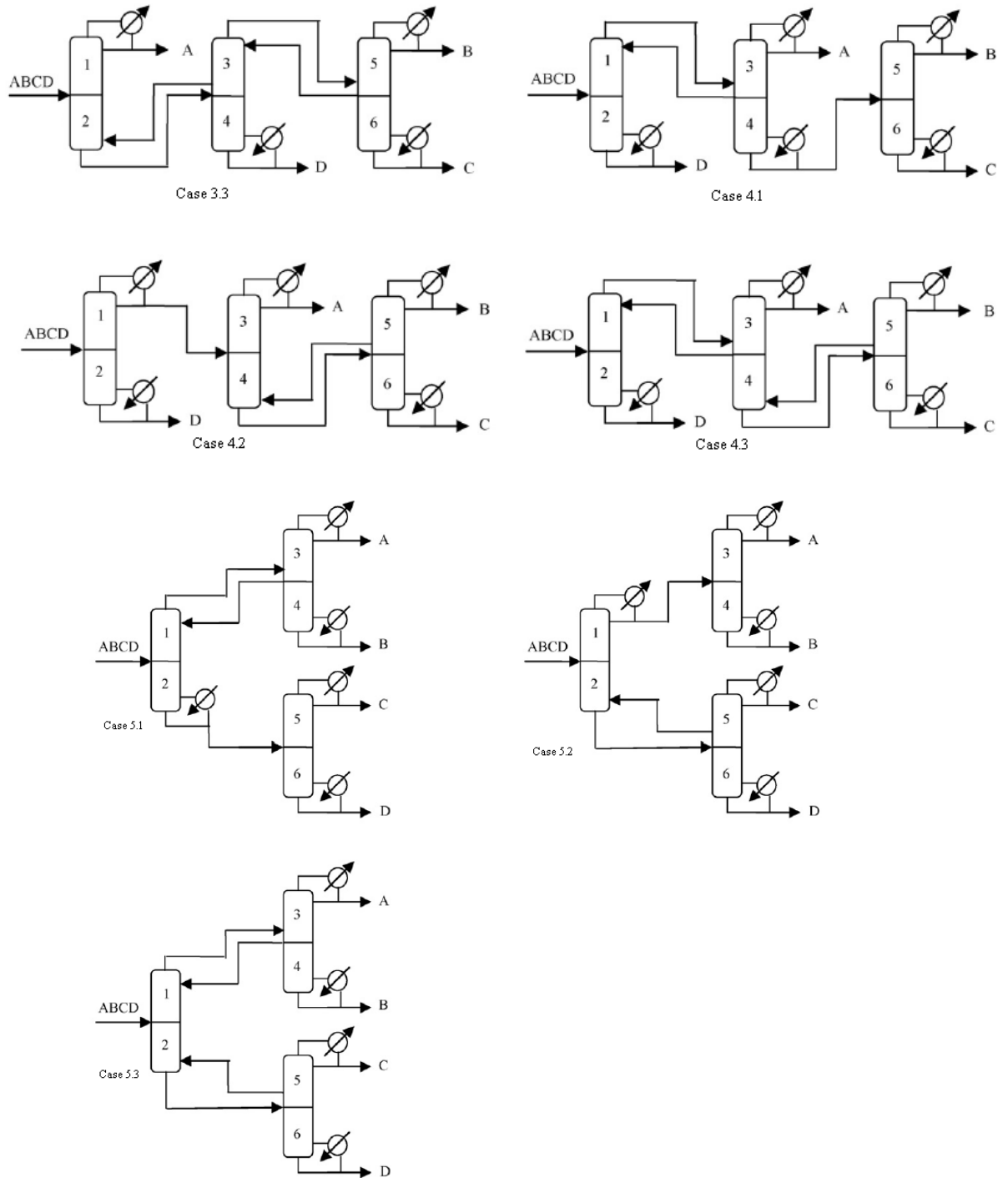


Fig 11. (Continued)

The energy requirements for the condenser and the reboiler for a sharp split in each column will be obtained for 25 trays, then we will be able to compare the simple distillation columns sequence with the thermally coupled configurations.

Table 10. Energy requirements for thermally coupled configurations.

	<b>Case 1.1</b>			<b>Case 1.2</b>		
	Col1.	Col2.	Col3.	Col1.	Col2.	Col3.
<b>Energy condenser (kW)</b>	1842	655	906.8	1670	1022	708.4
<b>Energy reboiler (kW)</b>	-	2555	916.1	1703	-	1764
	<b>Case 1.3</b>			<b>Case 2.1</b>		
	Col1.	Col2.	Col3.	Col1.	Col2.	Col3.
<b>Energy condenser (kW)</b>	1844	666.6	616.6	-	1735	644.6
<b>Energy reboiler (kW)</b>	-	-	3193	1555	214	650.1
	<b>Case 2.2</b>			<b>Case 2.3</b>		
	Col1.	Col2.	Col3.	Col1.	Col2.	Col3.
<b>Energy condenser (kW)</b>	1131	-	2324	-	-	2882
<b>Energy reboiler (kW)</b>	1345	1302	1043	1509	558.9	861.8
	<b>Case 3.1</b>			<b>Case 3.2</b>		
	Col1.	Col2.	Col3.	Col1.	Col2.	Col3.
<b>Energy condenser (kW)</b>	1473	934.5	870.6	1659	-	1611
<b>Energy reboiler (kW)</b>	-	2460	878.5	1686	1193	444.7
	<b>Case 3.3</b>			<b>Case 4.1</b>		
	Col1.	Col2.	Col3.	Col1.	Col2.	Col3.
<b>Energy condenser (kW)</b>	1813	-	1459	-	2660	894.4
<b>Energy reboiler (kW)</b>	-	2846	486.7	1465	1242	902.1
	<b>Case 4.2</b>			<b>Case 4.3</b>		
	Col1.	Col2.	Col3.	Col1.	Col2.	Col3.
<b>Energy condenser (kW)</b>	1302	1807	635.2	-	2797	668.3
<b>Energy reboiler (kW)</b>	1335	-	2464	1464	-	2057
	<b>Case 5.1</b>			<b>Case 5.2</b>		
	Col1.	Col2.	Col3.	Col1.	Col2.	Col3.
<b>Energy condenser (kW)</b>	-	1990	918	1180	1427	683.4
<b>Energy reboiler (kW)</b>	1249	788.5	926.7	-	1431	1918
	<b>Case 5.3</b>					
	Col1.	Col2.	Col3.			
<b>Energy condenser (kW)</b>	-	2278	673.5			
<b>Energy reboiler (kW)</b>	-	1005	2004			

As before, the next step is comparing the costs of the distillation columns equipment and the costs of energy consumption. The costs of the distillation columns equipment (shell and trays) is the same as the simple distillation columns with 25 trays. However

the costs of energy consumption should be less, doing the same procedure as the case above we can obtain the next results:

Table 11. Heat exchangers cost evaluation for thermally coupled schemes

	Heat exchanger	UA	U,m <sup>2</sup>	Cap. Cost, \$
<b>Case1.1</b>	Con1.	315000	99.23	16051
	Con2.	63600	20.03	14742
	Con3.	55800	17.58	-
	Reb1.	-	-	31244
	Reb2.	177209	55.82	20446
	Reb3.	92297	29.07	76582
	Total			221.73
<b>Case1.2</b>	Con1.	286000	90.09	42646
	Con2.	99200	31.25	21428
	Con3.	43600	13.73	12558
	Reb1.	90214	28.42	20145
	Reb2.	-	-	-
	Reb3.	176656	55.65	31180
	Total			219.14
<b>Case1.3</b>	Con1.	315000	99.23	45409
	Con2.	64700	20.38	16231
	Con3.	37900	11.94	11465
	Reb1.	-	-	-
	Reb2.	-	-	-
	Reb3.	319315	100.58	45813
	Total			232.13
<b>Case 2.1</b>	Con1.	-	-	-
	Con2.	195000	61.43	33248
	Con3.	100000	31.5	21540
	Reb1.	133872	42.17	26037
	Reb2.	12074	3.8	5451
	Reb3.	29891	9.42	9825
	Total			148.32
<b>Case 2.2</b>	Con1.	120000	37.8	24250
	Con2.	-	-	-
	Con3.	407000	128.21	53639
	Reb1.	120369	37.92	24298
	Reb2.	75526	23.79	17948
	Reb3.	47487	14.96	13274
	Total			242.67

	<b>Heat exchanger</b>	<b>UA</b>	<b>U,m<sup>2</sup></b>	<b>Cap. Cost, \$</b>
<b>Case 2.3</b>	Con1.	585000	184.28	67904
	Con2.	-	-	-
	Con3.	-	-	-
	Reb1.	129008	40.64	25418
	Reb2.	31501	9.92	10166
	Reb3.	36953	11.64	11278
	Total		246.48	114766
<b>Case 3.1</b>	Con1.	252000	79.38	39278
	Con2.	72400	22.81	17461
	Con3.	89900	28.32	20100
	Reb1.	-	-	-
	Reb2.	233641	73.6	37394
	Reb3.	51486	16.22	13991
	Total		220.32	128224
<b>Case 3.2</b>	Con1.	289000	91.04	42937
	Con2.	-	-	-
	Con3.	175000	55.13	30990
	Reb1.	87089	27.43	19689
	Reb2.	107182	33.76	22533
	Reb3.	25581	8.06	8880
	Total		215.41	125028
<b>Case 3.3</b>	Con1.	310000	97.65	44940
	Con2.	-	-	-
	Con3.	150000	47.25	28035
	Reb1.	-	-	-
	Reb2.	266597	83.98	40743
	Reb3.	28809	9.08	9593
	Total		237.95	123310
<b>Case 4.1</b>	Con1.	-	-	-
	Con2.	509000	160.34	62031
	Con3.	91800	28.92	20375
	Reb1.	130828	41.21	25651
	Reb2.	59381	18.71	15350
	Reb3.	53155	16.74	14284
	Total		265.91	137691
<b>Case 4.2</b>	Con1.	125000	39.38	24902
	Con2.	346000	108.99	48266
	Con3.	64500	20.32	16198
	Reb1.	117288	36.95	23892
	Reb2.	-	-	-
	Reb3.	146864	46,26	27653
	Total		251.89	140911



	Heat exchanger	UA	U,m <sup>2</sup>	Cap. Cost, \$
<b>Case 4.3</b>	Con1.	-	-	-
	Con2.	535000	168.53	64073
	Con3.	68600	21.61	16860
	Reb1.	131490	41.42	25735
	Reb2.	-	-	-
	Reb3.	121623	38.31	24463
	Total		269.86	131130
<b>Case 5.1</b>	Con1.	-	-	-
	Con2.	59000	18.56	15286
	Con3.	353000	111.2	48899
	Reb1.	82025	25.84	18937
	Reb2.	34893	10.99	10865
	Reb3.	83842	26.41	19209
	Total		193.02	113195
<b>Case 5.2</b>	Con1.	148000	46.62	27792
	Con2.	273000	86	41376
	Con3.	43900	13.83	12614
	Reb1.	-	-	-
	Reb2.	63167	19.9	15980
	Reb3.	180092	56.73	31573
	Total		223.07	129334
<b>Case 5.3</b>	Con1.	-	-	-
	Con2.	436000	137.34	56093
	Con3.	43200	13.61	12483
	Reb1.	-	-	-
	Reb2.	44329	13.96	12694
	Reb3.	187244	58.98	32382
	Total		223.89	113652

### 3.2.3 Discussions

First of all, we compared distillation columns with 100 trays and 25 trays. The costs regarding to the equipment (column shell and trays) are larger in the first case, because the total height is an important factor which affects to the total cost. However the energy costs are less important in the infinite number of trays, because as we saw before, with infinite number of trays the energy required is minimum. If, for example, we compared the case 1 in terms of equipment costs and energy costs:

Equipment costs:

$$\left. \begin{array}{l} 100 \text{ Trays: } 247,283 \$ \\ \\ 25 \text{ Trays: } 85,412 \$ \end{array} \right\} \frac{247,283 - 85,412}{247,283} = 65\%$$

It implies 65% more costs in the first case than in the second one.

Energy costs:

$$\left. \begin{array}{l} 100 \text{ Trays: } 121,288 \$ \\ \\ 25 \text{ Trays: } 182,025 \$ \end{array} \right\} \frac{182,025 - 121,288}{182,025} = 33\%$$

In this case, the energy costs are larger for the second case, because as we discussed before, with infinite number of trays the energy required is minimum.

Secondly, we compared the simple distillation column configurations and thermally coupled configurations with the same number of trays (25) The results show that the costs in the thermally coupled configurations are less than for the simple distillation columns. This is because in thermally coupled schemes we get the same purification as the simple distillation columns but using less reboilers and/or condensers. They, as we saw before, are replaced by side streams.

If, we compare the case 1, the energy costs for the simple distillation columns and for the thermally coupled configurations:

Energy costs:

$$\left. \begin{array}{l} \text{Simple configuration: } 182,025 \$ \\ \\ \text{Thermally coupled (the best case): } 118,917 \$ \end{array} \right\} \frac{182,025 - 118,917}{118,917} = 35\%$$

With these results, we can conclude that thermally coupled configurations are a promising strategy to reach the scope of energy reduction, and therefore the energy costs.

## **4. Conclusion**

Thermally coupled distillation columns were presented as a new method to save energy for separations of multicomponent mixtures.

In this report, the simple distillation columns were compared with the thermally coupled configurations. For this purpose, distillation systems with less than  $N-1$  columns were studied, first considering the simple distillation columns in series and then the thermally coupled configurations.

A case study for the separations of four-component mixture showed the advantages of using thermally coupled configurations. Using Unisim, the reduction in the energy consumption and the cost reduction for the configurations could be illustrated.

## 5. Bibliography

- [1] Caballero J.A., Grossman I.E. Design of distillation sequences: from conventional to fully thermally coupled distillation systems. *Computers chem.Engng.*28, 2307-2329 (2004)
- [2] Iwakabe K.;Nakaiwa M.; Huang K.; Nakanishi T., Rosjorde A.;Ohmori T.; Endo A.; Yamamoto T. Energy saving in multicomponent separation using an internally heat-integrated distillation column (HIDic) *Applied Thermal Engineering* 26, 1362-1368 (2006)
- [3] Cheng H.C; Luyben W.L. Heat-integrated distillation columns for ternary separations. *Computers chem. Engng.*24, 707-713 (1985)
- [4] Errico M; Tola G.; Rong B.G, Demurtas D.; Turunen I. Energy saving and capital cost evaluation in distillation column sequences with a divided wall column. *Chemical Engineering research and design* (2009)
- [5] Errico M; Tola G.; Rong B.G, Demurtas D.; Turunen I. A method for systematic synthesis of multicomponent distillation with less than N-1 columns. *Computers chem.Engng.*48, 907-920 (2009)
- [6] Economic indicators. *Chemical Engineering* (2009)
- [7] Halvorsen. I.V. Minimum energy requirements in complex distillation arrangements (2001)
- [8] Perry R.H.; Green D.W.; Perry's chemical Engineers'Handbook. McGraw-Hill (1997)
- [9] Resertarits M.R; Lockett M.J; *Distillation*