

UNIVERSITAT POLITÈCNICA DE CATALUNYA

Department of Chemical Engineering

**ENERGY OPTIMISATION AND
CONTROLLABILITY IN COMPLEX
DISTILLATION COLUMNS**

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CHAPTER 2. DIFFERENT DISTILLATION ARRANGEMENTS FOR MULTICOMPONENT SEPARATIONS

2.1 Abstract

In this chapter, a general overview is given of different distillation arrangements for the separation of multicomponent mixtures. Specifically, the chapter is focused in the most relevant conventional and non-conventional arrangements for ternary separations. According to the literature, these arrangements are the simple column with sidestream, the direct sequence of columns, the indirect sequence of columns, the simple column with side rectifier, the simple column with side stripper, the Petlyuk Column, and the DWC. A steady state comparative analysis of these arrangements is developed, including thermodynamic properties, operation DOF, design DOF, and design procedures. Reversibility and thermal coupling are given special attention. These two properties make the Petlyuk Column and the DWC very attractive in terms of energy efficiency. The DWC is studied in detail and some aspects not sufficiently covered in the literature are further discussed and clarified. Different design procedures for the DWC are described. Furthermore, a new design procedure that uses three decision variables for design optimisation is proposed and its benefits reported.

2.2 Introduction

Multicomponent distillation theory has been studied for decades. The bibliography for multicomponent distillation arrangements is vast. In the following paragraphs, few selected works, significant in the evolution of the knowledge of non-conventional arrangements, are reported.

Petlyuk et al. (1965) explained that one of the fundamental properties of reversible distillation is that no more than one component is stripped out in each column section. This guarantees reversibility during mixing of streams at the feed location. Considering thermodynamic reversibility the scientific approach for the selection of optimal multicomponent distillation arrangements, the authors described different arrangements with reversible mixing of streams and studied their requirement of energy and work of separation. The Petlyuk Column,

thermodynamically equivalent to the DWC, was found very favourable in terms of energy consumption.

Fidkowski et al. (1986) studied the optimisation of the “thermally coupled system of distillation columns” (that was the name they used for the Petlyuk Column). They analysed the operation DOF of the Petlyuk Column and searched the values for boilup minimisation. Minimum vapour flow in the different column sections was calculated using the Underwood classic method (Underwood, 1948). Interestingly, a set of optimal solutions was found.

The same authors, (Fidkowski et al. 1987) studied the operation optimisation of the simple column with side stripper and the simple column with side rectifier. They compared the schemes with the Petlyuk Column and concluded that the Petlyuk Column has lower minimum energy consumption. They also concluded that the simple column with side stripper and the simple column with side rectifier have lower minimum energy consumption than the direct and indirect sequences.

Carlberg et al. (1989) developed a generalised approach to the Petlyuk Column analysis based on Underwood’s original work. They concluded that the Petlyuk Column, like other complex arrangements, is more favourable with respect to the first law and less favourable with respect to the second law of the thermodynamics. In other words, the Petlyuk Column takes a great advantage regarding the quantity of required energy, but if the temperature of the streams that provide the energy is regarded, the advantage of the Petlyuk Column diminishes. This is mainly due to having only one reboiler and one condenser.

Trinatafyllou et al. (1992) presented a design model and a design procedure for the DWC. The authors studied the optimisation of the DWC total cost (energy and investment costs). Two variables were used as decision variables for the design optimisation. This design optimisation procedure will be analysed and discussed in section 2.6.

2.3 Steady state analysis of a distillation process.

In chapters two and three, only steady state is considered. Although a dynamic analysis may indicate drastic restrictions with large effect on the cost of a distillation process, a steady state analysis permits to evaluate the distillation cost, at least in terms of energy and investment costs.

Assuming a distillation arrangement already selected, the steady state study of a distillation process includes two main stages, which are design and operation. One of the main tasks at the design stage is to determine the appropriate number of trays in each distillation section. A section is defined as a group of trays without any feed or product stream, and limited by trays which have a feed or a product stream. The main task at the operation stage it to determine the appropriate value of all the material and energy flows that are not given by the system. Although

design and operation are two separated stages, design methods assume specific operating conditions to evaluate the objective function.

2.3.1 Design stage

Distillation cost is normally the objective function to be minimised during the design stage. In this work, optimal designs are considered those designs that minimise the sum of energy and trays costs. Although the new trend is to integrate design and control, most design methods only consider the trade-off between energy cost and the cost of the trays. In chapters two and three, controllability aspects are not considered. However, in chapter seven, the relationship between DWC design and controllability is studied.

Many authors agree that the effect of the number of trays in the distillation cost is minimal compared to the energy cost, provided that very high pressures and corrosive components are not present (Glinos et al. 1988). Therefore, energy is the most important variable of the cost estimation. However, the cost of the trays should also be taken into account.

In the design of all distillation columns, there is a trade-off between the number of trays and the reflux ratios. Trays can be added in order to have lower boilups. Many design methods are based on calculations at minimum reflux conditions (infinite columns). Depending on the relative price of trays and energy, an optimal ratio of actual reflux ratio (RR) to minimum reflux ratio (MRR) is assumed, which corresponds to a specific number of trays. A widely extended example of such design methods for simple distillation columns consists in the shortcut equations of Underwood-Fenske-Gilliland (King, 1981).

In terms of investment costs, batch distillation provides the best method of separating multicomponent mixtures. For this reason, batch distillation is the most common mode of operation in production plants of small capacities. However, large capacities require continuous operation. As indicated, batch distillation is out of the scope of this thesis work.

2.3.2 Operation stage

When operation DOF are available for optimisation, energy minimisation is often considered. The objective function considered in this work is basically the boilup flowrate, or the sum of boilup flowrates, in arrangements with more than one reboiler. Therefore, optimal operation is the operation that minimises the boilup. The boilup is almost proportional to the required energy, which is usually the dominant factor in the total cost of a distillation plant.

The use of energy streams at different temperatures may reduce a lot the energy cost of a distillation process. This fact will be considered when comparing advantages and disadvantages of the different distillation arrangements.

2.4 Different distillation arrangements for multicomponent separations

In the literature, some arrangements for the separation of multicomponent mixtures have received special attention. They appear in the most relevant literature addressing comparisons between multicomponent distillation arrangements (Tedder et al., 1978), (Fidkowski et al., 1987), (Glinos et al., 1988) among others. These arrangements are:

1. The simple column with sidestream
2. The direct and indirect sequences of columns
3. The simple column with side rectifier and the simple column with side stripper
4. The Petlyuk Column and the DWC

All these distillation arrangements can be used for the separation of multicomponent mixtures in three products. Some of them are easily extended to distillation arrangements for the separation of n -component mixtures in n products. In this thesis work, the separation of ternary mixtures into three products is analysed with special attention. The components of these ternary mixtures are called A, B, and C, where A is the most volatile component, B is the component with mid volatility, and C is the less volatile component.

Of course, other arrangements of increased complexity can be proposed. However, following the literature trend, more complex arrangements are not considered in this thesis. On the other hand, variations such as intermediate reboilers and condensers and heat integration may improve the performance of some of the arrangements.

Heat integrated distillation arrangements present some energy exchange between a reboiler and a condenser of different columns of the arrangement, providing an exergy minimisation. The number of possible heat integrated distillation arrangements is constrained by the second law of the thermodynamics since the temperature of the heat stream rejected by the condenser must be high enough to ensure heat transfer with the reboiler that reuses this heat. Reboiler and condenser temperatures can be matched by adjusting the pressures in the distillation columns. However, practical limitations occur when large pressure changes are required in order to have the heat streams at the appropriate temperatures. Pressure increase may be inadequate due to practical reasons as reboiler fouling. The column sequences can be energy integrated but normally, one of the two columns will have to operate at a higher pressure in order to provide the temperature driving force required for heat integration. The Petlyuk Column and the DWC, which have only one condenser and reboiler, can not present energy integration.

To properly compare distillation cost of different arrangements for the separation of multicomponent distillations, energy integration of all the arrangements should be considered. But energy integration is out the scope of this work. Comparisons between heat integrated distillation arrangements can be found in Cheng et al. (1985) and Annakou et al. (1996). From

the conclusions of these works it is clear that, even though energy integration may reduce the energy requirement of conventional schemes, because of energy integration limitations, non-conventional arrangements are still preferable in many cases.

2.4.1 Simple column with sidestream

A simple column with a sidestream is the simplest arrangement for the separation of ternary mixtures. It consists of a simple column with one reboiler and one condenser, which has a sidestream for the removal of the mid product. The sidestream stage may be over the feed tray or below the feed tray (see Figures 2.1 and 2.2).

The number of sections of a distillation arrangement can be seen as the number of design DOF because the number of trays of each section can be chosen at the design stage. A simple column with side stream has three sections.

Different models, with their simplifications and detail consideration, may regard different number of operation DOF for the same distillation arrangement. The number of operation DOF given in this chapter corresponds to columns where heat condition of all the material streams is fixed at saturated liquid or saturated vapour. The specific model assumptions are described in section 4.3.1. For all the distillation arrangements except precisely the simple column with sidestream, A, B, and C product purities are considered specifications. Because of that, in this chapter, when computing the number of operation DOF of the different arrangements in order to compare them, three DOF are already removed. The simple column with side stream does not present any operation DOF. In fact, it could be said that it has a negative operational DOF because the composition of the three products can not be specified.

In the case of a sidestream column with the sidestream below the feed (Figure 2.1), a primary separation is performed in the two sections that are adjacent to the feed tray. This primary separation is the A-BC separation, which can be carried out to any desirable extent. Thus, any desired composition of A in the top stage (NT) and in the sidedraw stage (NS) can be achieved. In the section below the sidedraw stage, C is purified. The purification of C can be carried out to any desirable extent. However, there is a maximum concentration of B and a minimum concentration of C in the sidestream product, which is attained if the number of trays between the sidedraw stage and the bottom stage is infinite. Therefore, any purity of C in the bottoms product or any recovery of B in the sidestream can be specified but the sidestream purity can not be arbitrarily specified. A similar case occurs with a sidestream column with the sidestream over the feed tray. The composition of the sidestream product can not be specified at any value.

Vapour sidestream in columns with the feed over the sidestream (Figure 2.1) and liquid sidestream in columns with the feed below the sidestream (Figure 2.2) are the richest in the middle component. However, there is also incentive for taking a liquid sidestream below the

feed. Purity can be lost but the vapour rate required is drastically reduced and therefore the column is cheaper.

The design of sidestream distillation columns was studied by Glinos et al. (1985).

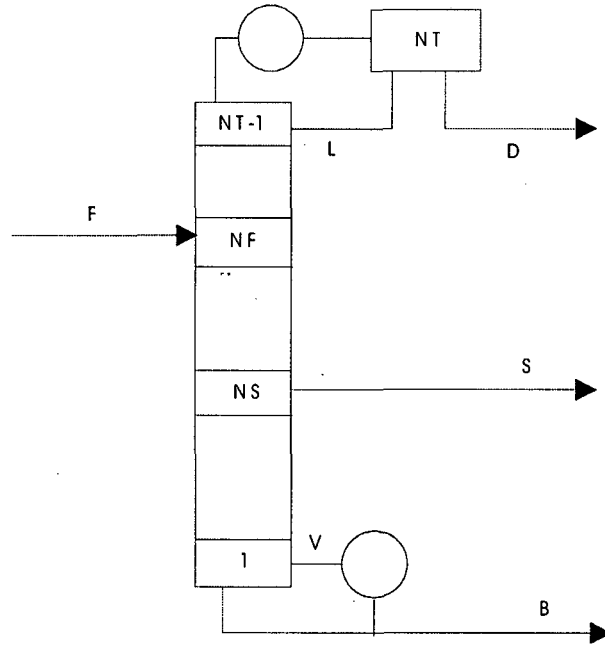


Figure 2.1: Sidestream column with sidestream below the feed

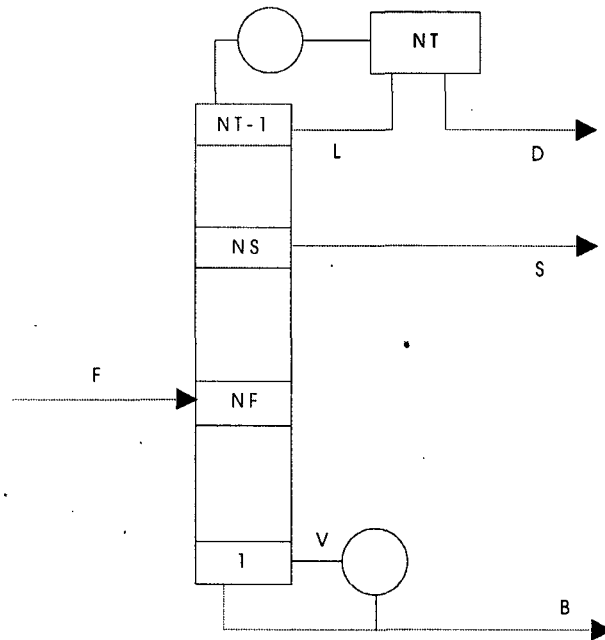


Figure 2.2: Sidestream column with sidestream above the feed

To show the composition profiles into a simple column with a sidestream, the separation of a mixture with constant relative volatilities $\alpha_A=4.65$, $\alpha_B=2.15$, and $\alpha_C=1$, or in other words, $\alpha=(4.65:2.15:1)$, is chosen as example. These relative volatilities could be representative for a mixture of benzene, toluene, o-ylene. A sidestream column with the feed stage below the sidedraw stage is chosen. Its design has $NT=28$, $NF=9$ and $NS=15$. The feed is an equimolar mixture of saturated liquid. All products are saturated liquid streams. A and C purities are specified at 0.99 molar composition and B purity, at 0.92 molar composition.

The model used to calculate the steady state is described in section 4.3.1. According to it, the boilup rate necessary for this separation is $V=4.38$ kmol per kmol of feed. In Figure 2.3, liquid composition profiles are shown. Notice that the sidestream product is in the tray where the B composition is maximum, which is tray $NS=15$. A B product purity of 0.99 molar is not achievable. If a purity larger than 0.92 is required, the boilup increases sharply.

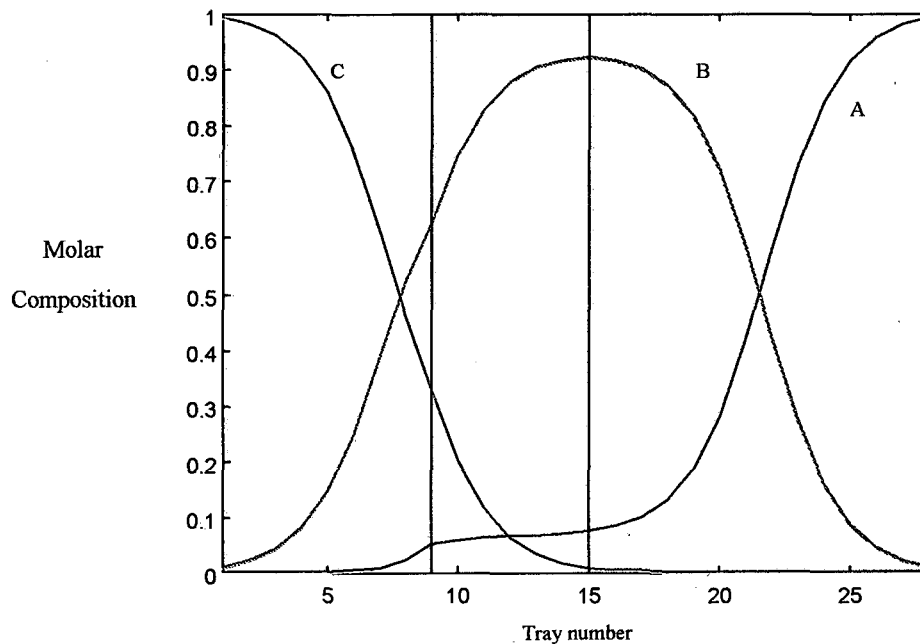


Figure 2.3: Composition profiles in a sidestream column

Not all the desired product compositions can be achieved by this arrangement. However, in those cases in what the desired purity can be achieved, the simplicity of this arrangement makes it desirable. Consequently, it is an interesting arrangement when the required B purity is not high.

2.4.2 Direct and indirect column sequences

The direct and indirect column sequences are also called direct and indirect trains of columns. They consist of two simple distillation columns connected in such a way that one product of the

first column is the feed of the second column. In the literature, they are considered to be the conventional arrangements for ternary distillations. These arrangements have four sections, two sections in each one of the simple columns. The number of operational DOF in the direct and indirect trains of columns is one.

The direct column sequence consists of a simple column that carries out the A-BC separation, connected to another simple column at the bottom stage. The downstream column carries out the B-C separation (see Figure 2.4). The indirect train carries out first the AB-C separation in a simple column, which is connected to another simple column at the distillate stage. The downstream column carries out the A-B separation (see Figure 2.5). The trains of columns are able to separate the ternary mixtures into products of any desired purity.

For an optimal direct sequence, the connecting stream is boiling liquid. In the same manner, for an optimal indirect sequence, the connecting stream is saturated vapour. In this work, these are the considered heat conditions of the connecting streams (as explained, stating that the number of operational DOF in the column sequences is one, the DOF associated to the heat condition of the connecting streams is not computed).

To design the sequences of columns is simple. Shortcut methods for simple columns can be applied to determine the optimal design of every column. Two specifications are required by the shortcut equations to calculate the optimal number of trays of every column. Typically, in a direct train, A purity and A recovery in the distillate are specified for the design of the first column, and purity of B and C are specified for the design of the second column. As it is assumed that it is not specified, the A recovery in the distillate of the first column is a design decision variable, which could be used for optimisation. However, its value is well limited because all A entering the second column will appear in the mid product.

To show the composition profiles into a direct train of columns, the separation of the same mixture in section 2.4.1 with $\alpha=(4.65:2.15:1)$ is chosen as example. Feed is an equimolar mixture of saturated liquid, all products are saturated liquid streams, but in this case, the required purity of all three products is 0.99 molar. To calculate the steady state, model assumptions described in 4.3.1 are also used. This separation problem, with the same model assumptions, will serve as example in the coming sections for the other distillation arrangements.

To show the best of the distillation arrangement, the optimal design is selected. The number of trays of every column is found assuming that the energy/investment cost trade-off is solved at $RR/MRR=2$. Optimal design has $NTI=18$, $NTII=19$, $NFI=10$ and $NFII=9$. Also optimal operation is selected (the operation DOF is chosen to minimise the boilup). At optimal operation, the sum of the two boilups is $VI+VII=3.58$ kmol per kmol of feed. In Figures 2.6 and 2.7 the composition profiles into the first and the second columns of the direct train of columns can be seen. Notice that the composition of B in the first column achieves a maximum in tray 5.

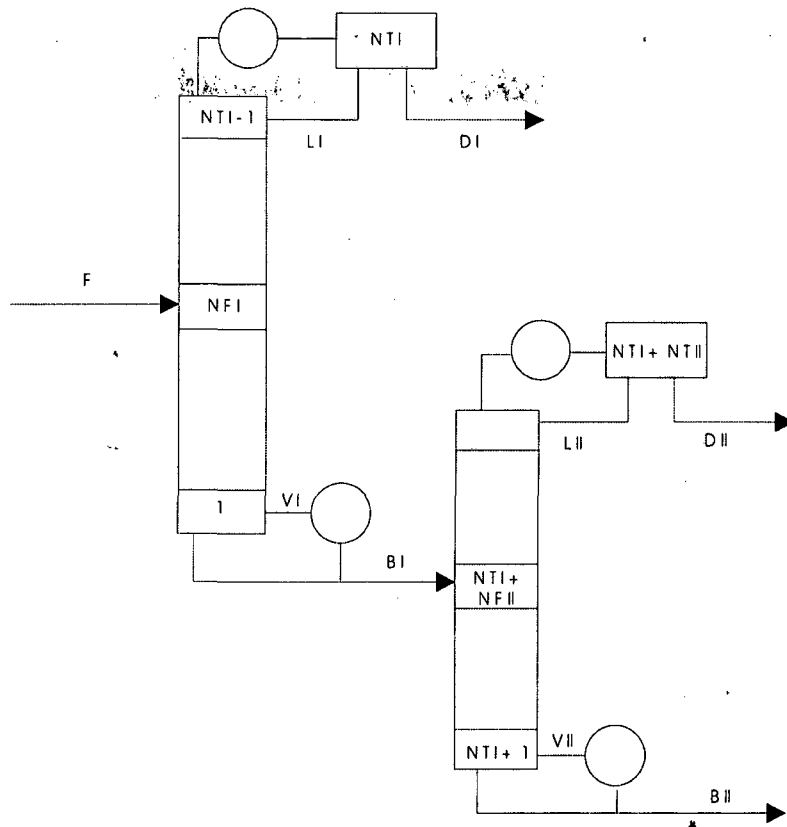


Figure 2.4: Direct sequence of columns

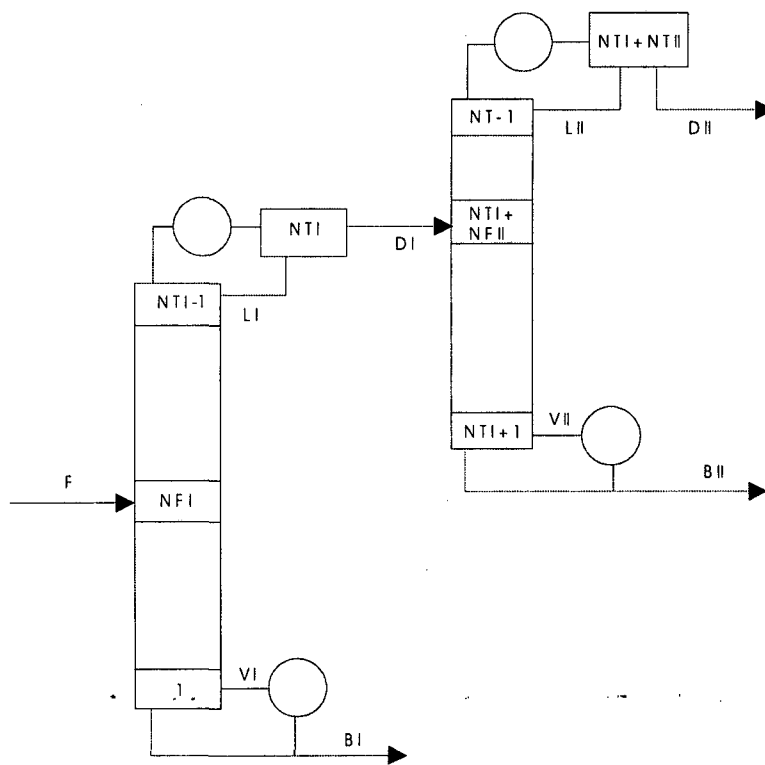


Figure 2.5: Indirect sequence of columns

For the same separation example, and with $RR/MRR=2$, the optimal design of the indirect sequence of columns has $NTI=18$, $NTII=19$, $NFI=9$ and $NFII=10$. The optimal operation has $VI+VII=3.28$ kmol per kmol of feed. This boilup is lower than the boilup of the optimal direct sequence. In Figures 2.8 and 2.9, the composition profiles into the first and the second columns of the indirect sequence can be seen. The composition of B has a maximum in tray 15 of the first column.

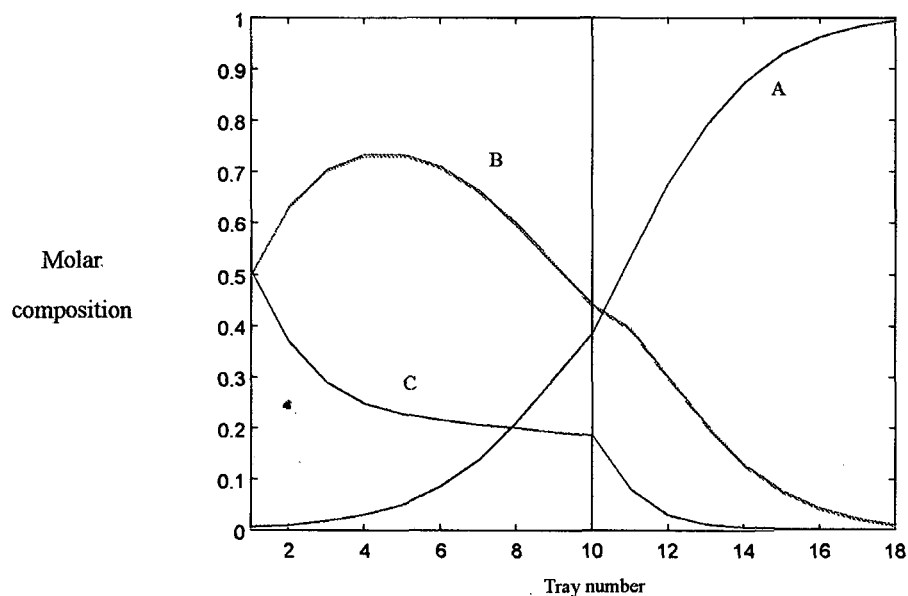


Figure 2.6: Composition profiles in the first column of a direct sequence

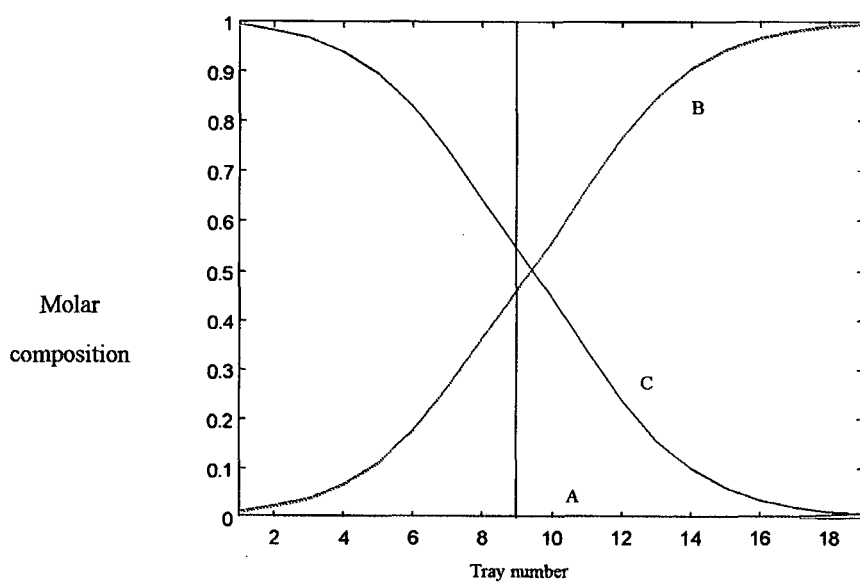


Figure 2.7: Composition profiles in the second column of a direct sequence

In any column sequence, at the extreme having a non-final product of any column, a remixing of components occurs. Consider a ternary mixture being separated in a direct train. The bottoms product of the first column contains mainly B and C. The quantity of A is so small that it has no influence. Since B is more volatile than C, ascending through the trays immediately above the bottom tray, the composition of B increases while the composition of C decreases. Only when component A begins to have an important role because of a considerable composition, the compositions of B and C decrease as the composition of A increases. Because of that, a maximum of B composition occurs in some tray between the bottom and the feed. The fact that the composition of B has a higher value in a tray different from the product tray is known as remixing effect. Remixing is a source of inefficiency, which can not be avoided in a train of columns. In Figures 2.6 and 2.8, the B composition maximum is clearly seen.

Simple column sequences are easily extended to arrangements for the separation of multicomponent mixtures into pure products. The number of columns of the sequence needed for the separation of an n -component mixture is $n-1$. Each of the columns separates one of the two extreme components from the rest. Thus, the key components of all the columns of a train of columns are the two lighter or the two heavier components. As has been seen, the separation of ternary mixtures requires two columns. In a direct sequence, the key components of the first column are A and B, and the key components of the second column are B and C. In an indirect sequence, they are B and C in the first column, and A and B in the second column.

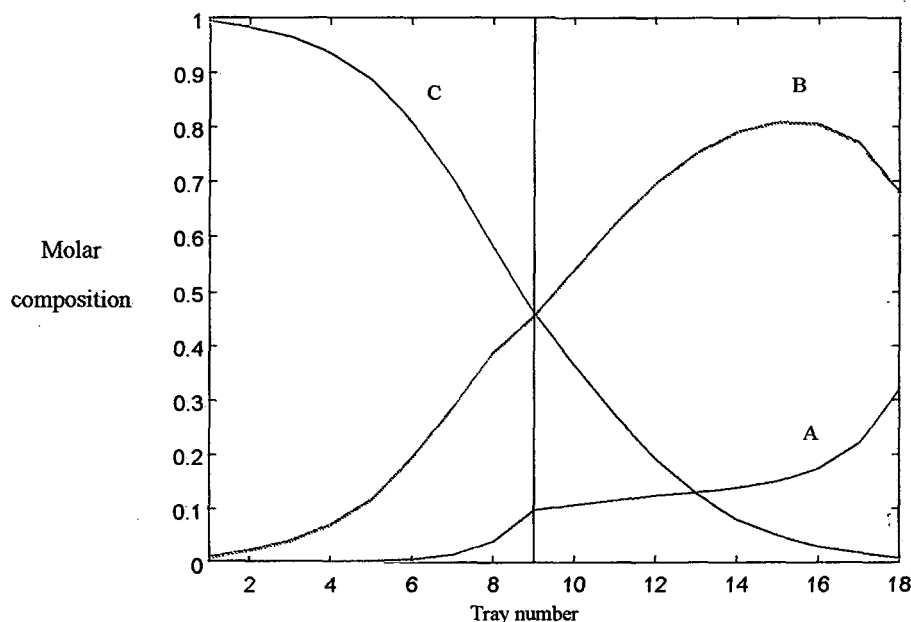


Figure 2.8: Composition profiles in the first column of an indirect sequence

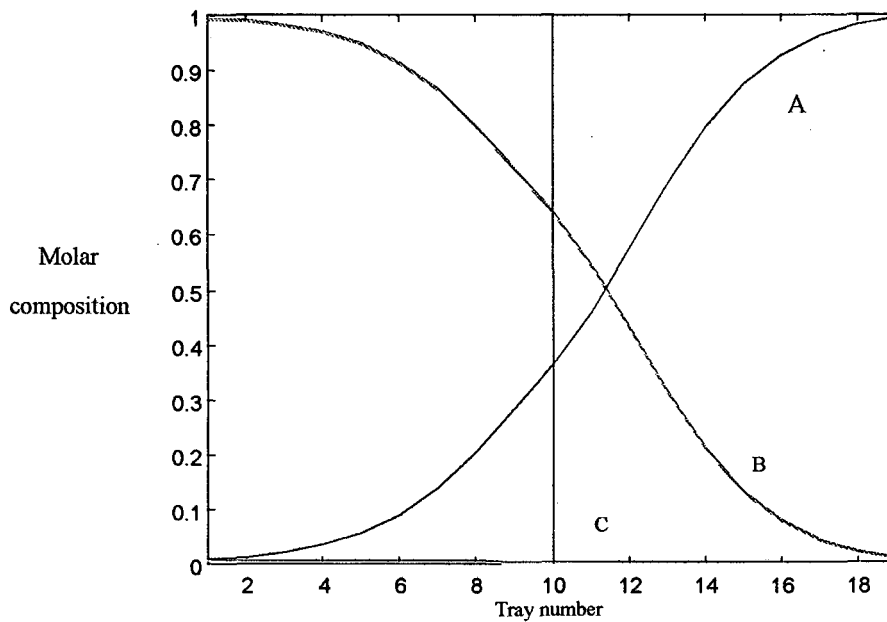


Figure 2.9: Composition profiles in the second column of an indirect sequence

2.4.3 Column with side rectifier and column with side stripper

Columns with side rectifier or side stripper are very interesting options for the separation of ternary mixtures. They are simple columns with a sidestream connected to a side section. This added section is a rectifier (simple column with side rectifier) or a stripper (simple column with side stripper). The number of sections of a column with side stripper or side rectifier is four. The number of operation DOF is one.

The column with side rectifier consists of a simple column with a sidestream connected to a side rectifier (see Figure 2.10). In the sections adjacent to the feed, A-BC separation is performed to any desired extent. In the lower section of the first column, C is purified to any desired extent. The rectifier purifies product B to any desired extent. The column with side stripper consists of a simple column with a sidestream connected to a side stripper (see Figure 2.11). In the sections adjacent to the feed, AB-C separation is performed to any desired extent. In the upper section of the first column, A is purified to any desired extent. The stripper purifies B to any desired extent. Therefore, any specified recoveries or purities in the three products can be attained in both, a column with side rectifier and a column with side stripper.

Columns with side stripper and side rectifier present thermal coupling at the connection between the main columns and the added section. In section 2.5.5, properties of thermal coupling will be analysed.

Design of columns with side strippers or side rectifiers can be essentially done the same way as the design of the column sequences (Finn, 1993). The sections of a column sequence and the

sections of a column with side stripper or side rectifier are equivalent in the sense that the same separations are performed in them. In Figure 2.12, schematic arrangement drawings show the equivalence between a direct train of columns and a column with side rectifier. In sections I and II, A-BC separation is performed. In sections III and IV, B-C separation is performed. In spite of this equivalence, the trains of columns do not have thermal coupling as the columns with side stripper or rectifier do. Consequently, to design a column with side stripper or side rectifier, the optimal design of the corresponding train of columns can be used as first approach. Then, design has to be adjusted to find out the actual optimal design.

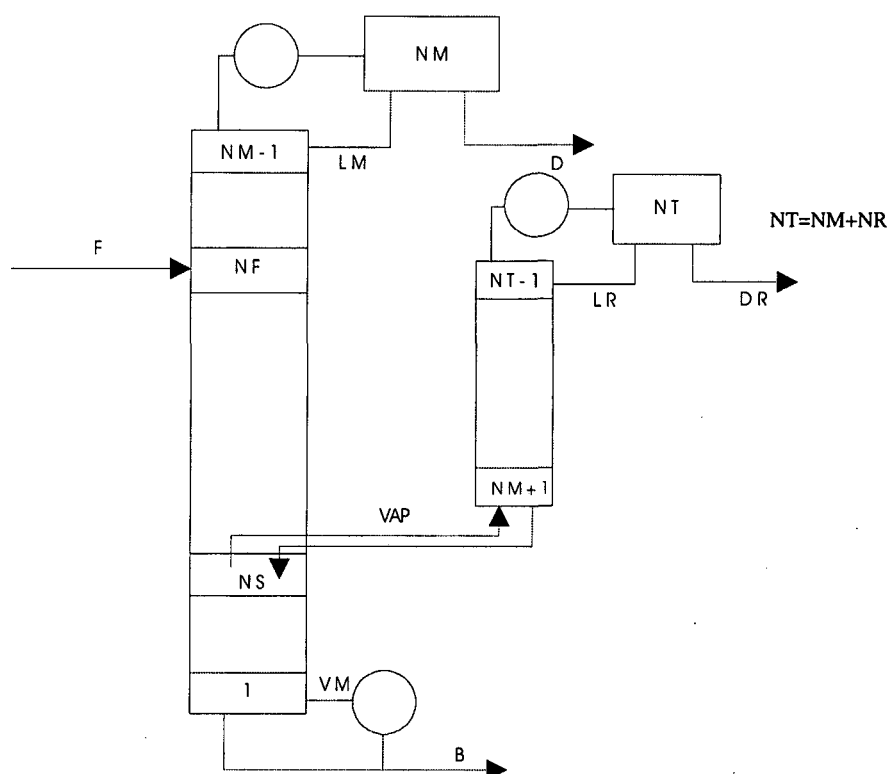


Figure 2.10: Column with side rectifier

The separation example in the previous section is taken again to show the composition profiles into a column with side rectifier. The optimal design is chosen, which has $NM=28$, $NR=9$, $NF=20$ and $NS=9$. Optimal operation has also been selected. The minimum boilup is $VM=3.27$ kmol per kmol of feed. This is a lower consume than the column sequences. In Figure 2.13, composition profiles are shown. Solid lines correspond to the composition profiles into the main column and dashed lines to the composition profiles into the rectifier. It can be seen that into the main column, B composition has a maximum in tray 12, which is not the sidedraw tray.

For the same separation example, in Figure 2.14, composition profiles into a column with side stripper are shown. Solid lines are the composition profiles into the main column and dashed

lines are the composition profiles into the stripper. The optimal design is chosen, which has $NM=28$, $NSTRIP=9$, $NF=9$ and $NS=19$. The operation has been also optimised. The sum of the main column boilup and the stripper boilup $VM+VS= 3.05$ kmol per kmol of feed. Notice that the column with side stripper has a lower boilup than the column with side rectifier.

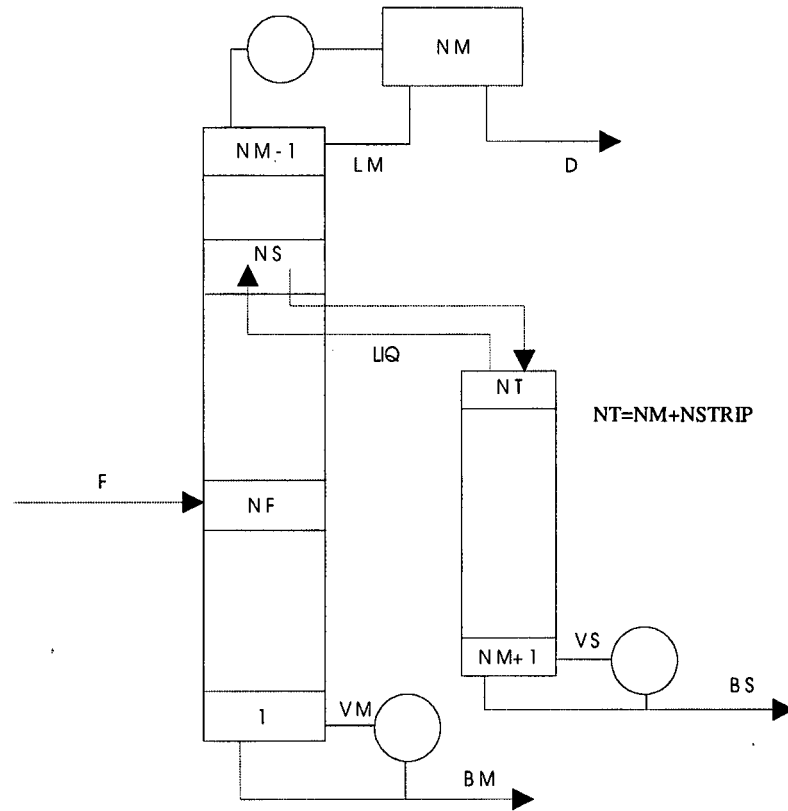


Figure 2.11: Column with side stripper

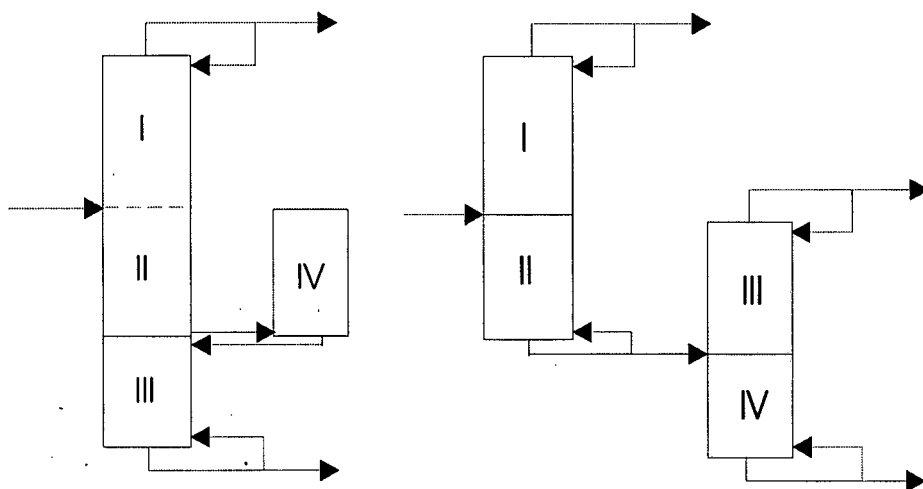


Figure 2.12: Equivalence between sections of a column with side rectifier and a direct sequence

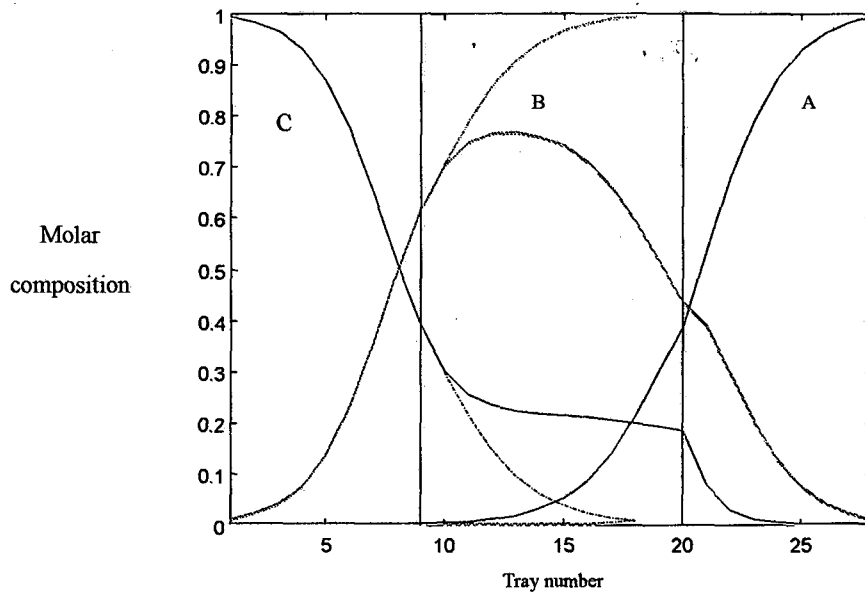


Figure 2.13: Composition profiles in a column with side rectifier

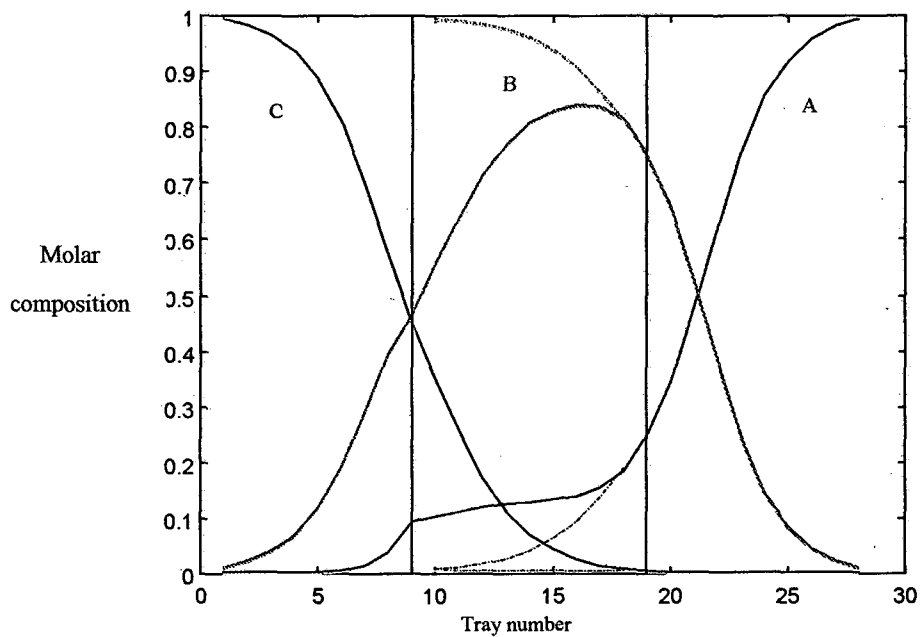


Figure 2.14: Composition profiles in a column with side stripper

In the examples, it is seen that the remixing effect is not avoided in the columns with side rectifier or side stripper, contrarily at what happened in the column with sidestream. In the column with side stripper, for instance, to avoid remixing effect, NS should be lower but in this

case, the composition of C in *NS* would be important, what is not possible because the entire C entering the stripper will appear in *BS*. A similar case occurs in a column with side rectifier.

2.4.4 The Petlyuk Column and the Divided Wall Column

In this thesis work, special attention is given to the Petlyuk Column and the DWC. Chapters four to seven deal with these distillation arrangements exclusively. The Petlyuk Column is a non-conventional arrangement for the separation of ternary mixtures which consists of a prefractionator connected to a main column at both ends. The prefractionator separates the lightest component A from the heaviest component C, while the middle component B is distributed, increasing the reversibility of the separation system in comparison with conventional arrangements. The main column separates A from B in trays above the middle stream product, and B from C in trays below the middle stream product. The main column has the three product streams and supplies the reflux and vapour streams required by the prefractionator, resulting in a double thermal coupling between both parts (see Figure 2.15 a). The Petlyuk Column has 6 sections and two operational DOF.

The DWC can be considered as thermodynamically equivalent to the Petlyuk column, although they have a very different external aspect (see Figures 2.15 a and b). The DWC is built in only one shell and a vertical wall divides its core in two parts that work as the prefractionator and the main column of the Petlyuk column, respectively.

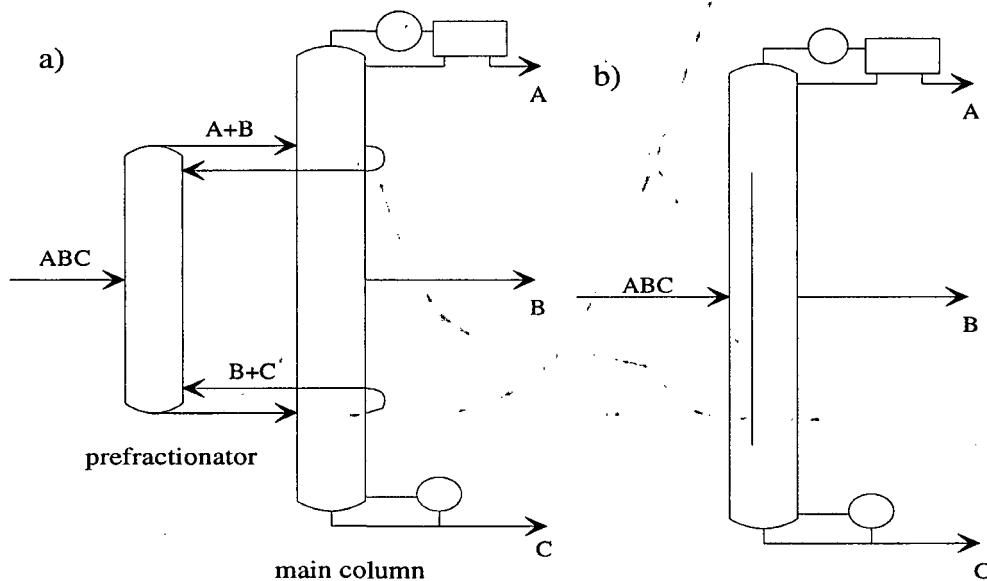


Figure 2.15: The Petlyuk Column (a) and the Divided Wall Column (b)

The split variables are characteristic of the DWC. *SPLITD* is defined as the ratio of the liquid descending through the main column to the total liquid arriving the top of the wall, and *SPLITB*

is defined as the ratio of the vapour ascending through the main column to the total vapour arriving the base of the wall. In Figure 2.16, a more detailed DWC drawing is shown. The DWC has a total number of trays of NT , NP trays in the prefractionator and NM trays in the main column. In the prefractionator, NF is the feed tray. In the main column, NCB is the last common tray before the wall, NS is the sidestream tray, and NCD is the first common tray after the wall. The condenser is a total condenser and the reboiler drum (considered to be in the base of the column) vaporises the liquid to be introduced in the column as boilup. Therefore, the reboiler is the first separation stage and NM is the last separation stage. Section 2.6 deals with the design of this distillation arrangement.

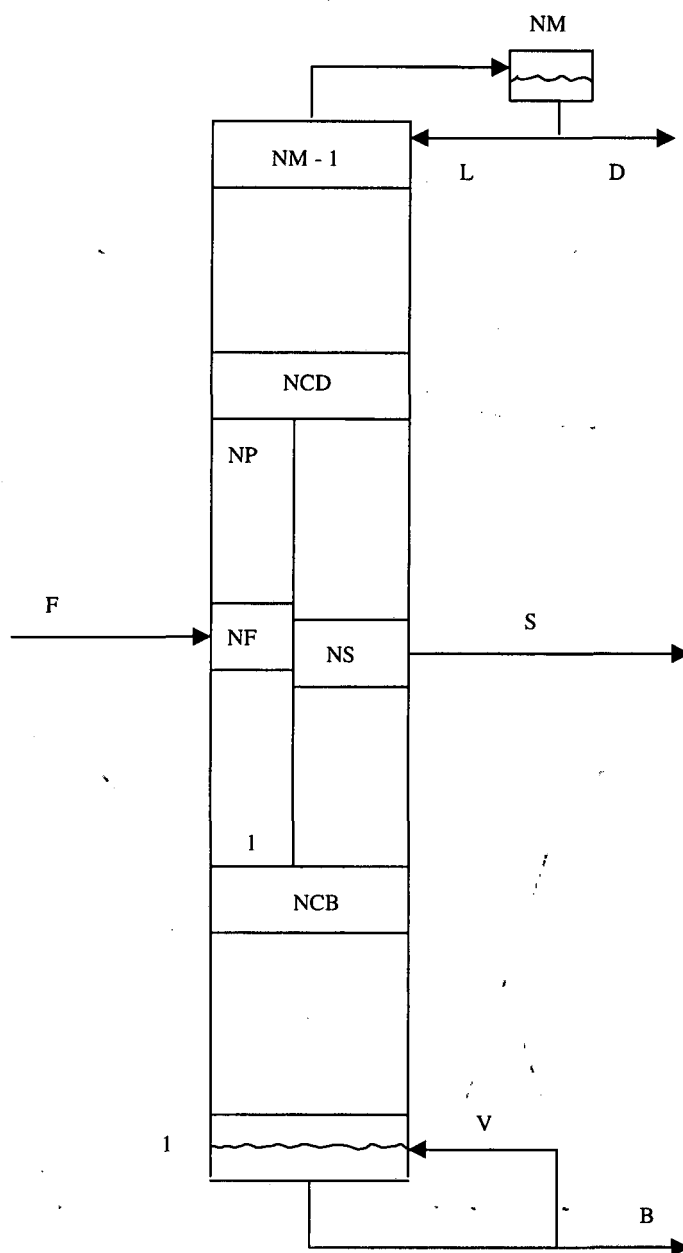


Figure 2.16: The Divided Wall Column

In Figures 2.17 and 2.18, the composition profiles into a DWC are shown for the separation example in the previous sections. The distillation is carried out in an optimally designed DWC with optimal operation (both operation DOF have been used to minimise the boilup). According to the design method in section 2.6.2, and with $RR/MRR=2$, optimal design has $NM=33$, $NP=13$, $NF=7$, $NS=17$, $NCD=26$, and $NCB=8$. Optimal operation has boilup $V=2.65$ kmol per kmol of feed, which is the lower boilup of all the arrangements. In Figure 2.17, it can be seen that B composition has two maximums in the prefractionator, approximately in trays 4 and 11.

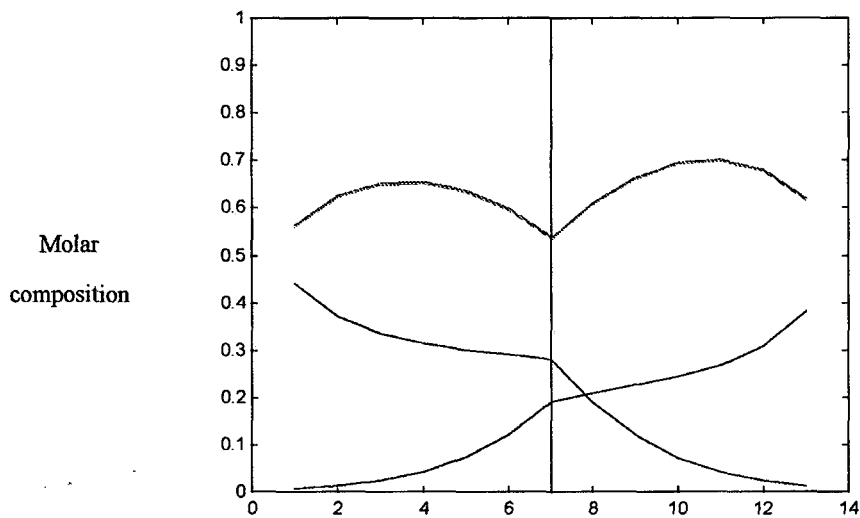


Figure 2.17: Composition profiles in the prefractionator of a Petlyuk Column

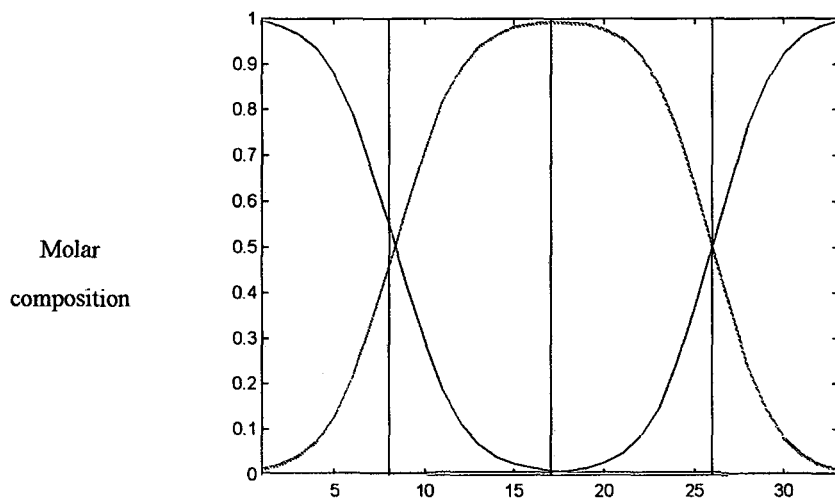


Figure 2.18: Composition profiles in the main column of a Petlyuk Column

Given the importance of the reversibility and thermal coupling characteristics of the Petlyuk and the DWC, in section 2.5, they will be better analysed.

2.4.4.1 The remixing effect in the Divided Wall Column

All separation processes consist in the removal of entropy of mixing from the feed. When a component has a higher composition in one tray different from the tray in what it is removed, part of the entropy removed is incorporated again. This effect is called remixing and it is a source of inefficiency. As has been seen in Figure 2.3, in a simple column with sidestream, remixing of B can be avoided. However, remixing can not be avoided in the rest of analysed arrangements, if high purity of products is required. In the first column of a column sequence, remixing appears because the residual component in the connection stage has necessarily a very small composition. In a column with side rectifier or stripper, remixing also appears. If the stage with maximum B has too much residual component, connection between columns can not be at this stage. Triantafyllou et al. (1992) explained the remixing effect in a Petlyuk Column and stated that in a Petlyuk Column, the remixing effect can be avoided. However, in the work, no explanation is given to justify the declaration. The results found in this work contradict the conclusion of Triantafyllou et al. (1992). The remixing effect can not be avoided in the prefractionator of the Petlyuk Column for the same reason why it can not be avoided in the columns with side rectifier or stripper. To obtain a pure B product, the composition of residual components in the extremes of the prefractionator is necessarily small, and this makes B composition increase in trays below the top of the prefractionator and in trays above the prefractionator bottom.

As has been seen, even if both operation DOF are used for energy minimisation, the DWC presents remixing. Even if the design DOF as well as the operation DOF are used to optimise the DWC, it presents remixing. Profiles in Figure 2.17, which correspond to an optimised DWC at optimal operation, show this.

2.4.4.2 Extension of the Petlyuk and the DWC schemes

The idea of the Petlyuk Column and the DWC can be extended to arrangements for the separation of multicomponent mixtures with more than three components. General DWC schemes are characterised by the following characteristics:

1. The total number of sections required for separating an n -component mixture is equal to $n*(n-1)$, instead of $2*(n-1)$ for the conventional sequences of columns.
2. It is sufficient to have only one condenser and one reboiler, independently of the number of components to be separated. In conventional distillation, each column of the sequence has a reboiler and a condenser.

3. The key components in each column are not two adjacent ones, as in conventional distillation, but the ones with extreme volatilities.
4. The n products are products of the main column. Contrarily, each column of a conventional arrangement has one final product and one connecting product.

The basic principle of vertical partitions can be extended from ternary mixtures to n -component mixtures. The addition of new partitions in theory permits the separation of feed streams into any number of pure fractions. But in practice, the number of fractions is naturally limited. An increasing number of components requires more theoretical trays and, with respect to the height of the column, imposes limitations on the pressure drop and produces undesirably high bottom temperatures.

2.4.5 Two other arrangements

An arrangement usually treated in the literature is the prefractionator arrangement. It is similar to the Petlyuk Column, but with simple connections (instead of thermal coupling connections) between the prefractionator and the main column. It requires two more exchangers, one at each prefractionator extreme. Another arrangement is considered in some important works. It is a Petlyuk Column that has the main column divided in two different columns. The sidestream tray is the division point. Compared to the Petlyuk Column, two more heat exchanges are also required by this arrangement, which are a reboiler and a condenser at the division point. Both arrangements are less energy efficient than the Petlyuk column, but can use energy of lower quality at the added exchangers, which is an advantage in terms of exergy.

2.4.6 Recollection

In Table 2.1, some characteristics of the different analysed arrangements are recollected.

Table 2.1: Characteristics of the analysed arrangements

	Side stream column	Direct sequence - indirect sequences	Side stripper - Side rectifier	DWC - Petlyuk Col.
Num. Sections	3	4	4	6
Num. Operation DOF	-1	1	1	2
Remixing	NO	YES	YES	YES

2.5 Distillation reversibility

Thermodynamically, the distillation process consists of the removal of entropy of mixing. The process requires exergy or work of separation, which is provided by the input and the removal of heat at different temperature levels. Heat at high temperature is fed in the reboiler and heat at low temperature is removed in the condenser. Efficiency of distillation columns is very low because the actual exergy needed for a separation is much larger than the exergy for reversible separation (Kaibel et al., 1990). Reversible distillation is not practically attainable. Besides, only some product compositions can be obtained in a reversible multicomponent distillation (Agrawal et al. 1996). However, in any distillation process, the reversibility study is important for the improvement of the efficiency. Obtaining a separation process of good thermodynamic quality, which is a process with minimum irreversibilities, requires the following points:

1. Sufficient number of theoretical plates
2. Addition of intermediate heaters and coolers
3. Small pressure drop
4. Appropriate enthalpy of the feed
5. Direct heat and mass transfer: thermal coupling
6. Correct thermodynamic distillation sequence

2.5.1 Sufficient number of theoretical plates

It is well known that the increase of number of trays in a distillation column reduces the required energy flows. This is due to the reversibility associated to long columns. All distillation arrangements can have trays added in order to obtain more reversible distillations.

2.5.2 Addition of intermediate heaters and coolers

Intermediate heaters and coolers may also be added in all kind of arrangements. With intermediate heaters and coolers, the process becomes more reversible and is more economical because in the intermediate heat exchangers less expensive utilities (lower quality energy) can be used (Agrawal et al. 1996). Systems with small relative volatilities exhibit large vapour streams and small temperature differences between reboiler and condenser. In this case, intermediate reboilers and condensers can not offer great advantages. Systems with high relative volatilities, however, provide good possibilities for intermediate exchangers.

Regarding the required exergy, it has to be noticed that the Petlyuk Column has an important inconvenient. In this arrangement, the heat has to be supplied at the highest temperature (boiling

point of C) and rejected at the lowest temperature (boiling point of A). This makes the Petlyuk Column and the DWC less interesting when not only energy minimisation but also exergy minimisation is important. Agrawal et al. (1998 b) reported the practical consequences of this fact.

2.5.3 Small pressure drop

Small pressure drop in a distillation column makes the processes more reversible.

In the Petlyuk Column, there are important restrictions for the pressure drop. Since vapour has to flow from the main column to the prefractionator's bottom, and vapour has to flow from the prefractionator's top to the main column, the pressure drop in the prefractionator has to be smaller than in the trays of the main column between the feeds. Good control of the pressure profiles in these zones is crucial for proper operation. To avoid operation problems, Agrawal et al. (1998 a) proposed structural changes in the Petlyuk Column arrangement. Having the prefractionator and the lower section of the main column in one shell and the three upper sections of the main column in another shell, vapour flows from the first shell to the second in both connection points. It is only necessary to have a higher pressure in the first shell. Having the prefractionator sections and the upper section of the main column in one shell and the three lower sections of the main column in another shell, a similar case is obtained. Notice that the DWC, being built in only one shell and not having valves in the connecting points, has more pressure restrictions than the Petlyuk Column. The main problem is that the vapour split in the bottom of the wall will be given by the relative pressure drop between the last common tray and the two trays above it. To obtain a desired split, specific pressure drops in this zone are required. Therefore, appropriate technical solutions are needed to have the appropriate pressure in each side of the wall. All these restrictions make the pressure manipulation in a Petlyuk Column and in a DWC a difficult task.

In the trains of columns and in the side rectifiers and side strippers, since there is only one connection point between the two distillation shells that form the arrangements, the pressure restrictions are much simpler. It is only necessary that one distillation shell has a larger pressure than the other.

2.5.4 Appropriate enthalpy of the feed

Appropriate enthalpy of the feed is a requirement that affects the same way all the arrangements. A vaporisation of the feed can considerably reduce the reboiler load in case of high concentration of the low boiling component in the feed. Subcooled feeds are useful when the concentration of the light component in the feed is small (Kaibel et al., 1990).

2.5.5 Thermal coupling

The direct heat and mass transfer is known as thermal coupling. Specifically, it consists in the heat and mass transfer through the contact of material streams. Thermally coupled distillation systems are arrangements in what different columns are connected by liquid and vapour countercurrent streams. At some ends of upstream distillation columns, condensers or reboilers are eliminated and the liquid or vapour flows needed as refluxes are side streams of downstream columns of the distillation arrangement. Therefore, thermal coupling implies recycling because it implies a stream going back to upstream columns.

Thermal coupling is one of the characteristic features of the Petlyuk Column. However, it is not an exclusive characteristic of this arrangement. Columns with side rectifiers or strippers are also conceived with thermal coupling. In the case of the Petlyuk Column, there is thermal coupling at both ends of the prefractionator. Because of that, the arrangement is also called Fully Thermally Coupled Distillation Column by some authors. The columns with side rectifier or side stripper only have one thermal coupling connection. In Figure 2.19, there is a scheme of thermal coupling in the top extreme of a distillation column.

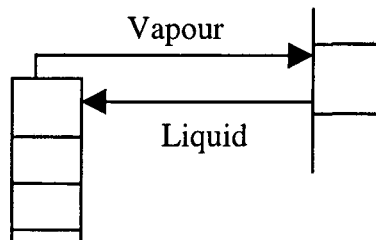


Figure 2.19: Thermal coupling in the top of a distillation column

One of the most important causes of exergy losses in distillation processes is the temperature difference needed for the heat transfer at the heat exchangers (Kaibel et al., 1990). The first advantage of thermal coupling is to avoid heat exchangers. But also important, thermal coupling permits a reversible mixing of streams at the end of the column that has lost the heat exchanger (Petlyuk et al., 1965).

There are not extra DOF because of the thermal coupling.

2.5.6 Correct thermodynamic distillation sequence

Finally, the correct thermodynamic distillation sequence is a very important characteristic of reversible distillations. According to reversibility, the correct thermodynamic distillation sequence is that in what no more than one component is stripped out in each section. In this case, reversibility during mixing of streams is guaranteed at the feed stage (reversible mixing occurs if

the feed composition is equal to the composition in the feed tray). The only arrangements with this characteristic are the Petlyuk Column and the DWC. In conventional distillation arrangements, as well as in columns with side rectifier or side stripper, the medium boiling component is forced in only one direction, either to the top or to the bottom of the distillation column. Because of that, the concentration of medium boiling component in the region of the feed tray is increased to values in excess of the feed concentration. This leads to a considerable increase in the entropy of mixing at the feed inlet (Kaibel, 1990).

2.6 Design procedures for the DWC

In the literature, few works consider the optimal DWC design. The design of the DWC, which involves the decision of the number of trays of its six sections, is a complex task. Only very simple models have been used for the design of complex distillation columns. A mathematical optimisation approach was presented by Dunnebieer et al. (1999) based on a detailed column model. Their approach was based on the use of superstructures coupled with mathematical optimisation, which allowed the simultaneous determination of both the design and the operational characteristics of the individual columns. However, their experience was that the approach was of limited use because mathematical problems could not be solved to global optimality.

The most reported work addressing the design of the DWC was written by Trinatafyllou et al. (1992). They presented a design model that provided a basis for investigating the DWC DOF, and explained how to use it in order to investigate the energy/investment costs trade-off. The model, which had been previously used as the basis for shortcut methods in the literature, consists of three simple distillation columns. It can be seen in Figure 2.20. In the work of Trinatafyllou et al. (1992), design DOF were determined through two decision variables. These decision variables were the recovery of A at the bottom of the prefractionator and the recovery of C at the top of the prefractionator. These two specifications, plus the product purity specifications, and shortcut calculations for the design of the three simple columns of the model were enough to determine the number of trays of all the sections. Fenske-Underwood-Gilliland equations were used for the shortcut calculations. Specifically, to determine the prefractionator design, A and C recoveries were specified and shortcut equations applied. To determine the design of COL2 and COL3, the required purity of products was specified and shortcut equations applied. This way, the optimal design for specified purity of products was searched in a two-dimensional plane, that of A and C prefractionator recoveries. Rules to guide the search were given and at the same time, a method for the optimisation of the DWC design was described.

Fidkowsi et al. (1986) studied the Petlyuk Column at minimum reflux ratio (infinite column). Therefore, design was not taken into account. However, the results of their work are very interesting for the Petlyuk Column design. The authors found an analytical solution of the

Petlyuk Column optimal operation, assuming ideal mixture, constant relative volatility, constant internal flow rates throughout the column, and separation into “almost pure” components. The variables chosen for operation optimisation were β and L_I . β is the fraction of component B in the top product of the prefractionator. Its expression is given in equation 2.1, where V_I is the vapour from the prefractionator’s top to the main column, L_I is the liquid from the main column to the prefractionator’s top, B is the quantity of B in the feed, x_B^I is the B liquid composition in the tray of the main column connected to the prefractionator top, and y_B^I is the B vapour composition at the top of the prefractionator.

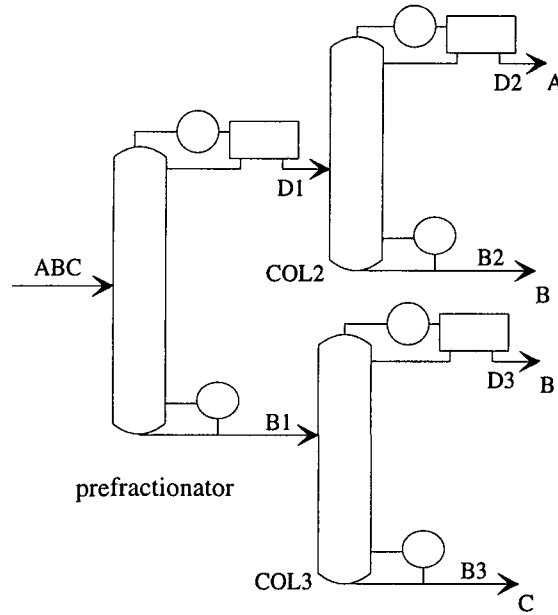


Figure 2.20: Design Model

$$\beta = \frac{V_I y_B^I - L_I x_B^I}{B} \quad (2.1)$$

Interestingly enough, an infinite number of solutions were found. The optimum values of β and L_I were contained in a closed section of the β - L_I plane. The values of β at the optimum are the values between β_P and β_R .

$$\beta_P = \frac{\alpha_B - \alpha_C}{\alpha_A - \alpha_C} \quad (2.2)$$

$$\beta_R = \frac{L_{II}^{opt} (\alpha_A - \alpha_B) - A \alpha_B}{L_{II}^{opt} \alpha_A - (L_{II}^{opt} + A + C) \alpha_C} \quad (2.3)$$

$$L_{II}^{opt} = \max \left(\frac{A\theta_1}{\alpha_A - \theta_1}, \frac{A\theta_2}{\alpha_A - \theta_2} + \frac{\alpha_B B}{\alpha_B - \theta_2} \right) \quad (2.4)$$

where the α are the relative volatilities of A, B, and C components; A , B , and C are the component flowrates in the feed, and θ_1 and θ_2 are the roots of Underwood's equation (Underwood, 1948).

β_p value has a special significance. Consider a simple column with a ternary mixture feed, and with sharp separation required between A and C. Consider the column is infinite. In this case, minimum boilup will happen when B has a pinch in the feed location. β_p is the value of B recovery in the distillate in this case, for which the energy consumption is minimal. β_p is called the preferred separation (Christiansen, 1997).

Since energy requirements are usually the dominant factor in the total cost of a distillation plant, results of this operation optimisation can serve as initialisations for the search of optimal designs.

Annakou et al. (1996) also studied the design of the DWC. They also used the simplified three-column model shown in Figure 2.20 as basis for shortcut designs. They investigate the role of β over the energy consumption and the annual cost of a DWC. They found that their optimal β values were close to β_p . They concluded that β is an important parameter for the design of the DWC.

In this work, two new design methods for the DWC are proposed, based on the design model of Figure 2.20. In the first one, two decision variables are used to determine the DWC design and in the second one, three decision variables are used to determine the DWC design. In both of them, rigorous simulations are involved.

2.6.1 Design procedure with two decision variables

In this section, a new design procedure is proposed. As the design procedure proposed by Triantafyllou et al. (1992), it considers two decision variables and is based on the simplified model shown in Figure 2.20. The main differences are that the procedure proposed here considers the β specification as decision variable, and involves rigorous simulations. The two decision variables used for optimisation are β and α , being α the A molar fraction in $B1$ (see Figure 2.20).

There are two basic differences between the DWC and the design model in Figure 2.20. The first one is the absence of thermal coupling in the model. As described in the previous section, thermal coupling is an essential element of the DWC that reduces its energy requirements. The second difference is that the model has the main column B divided in two columns: COL2 and COL3. Both differences cause that the simplified model exhibits larger energy requirement than the corresponding DWC. On the other hand, $B2$ and $D3$ replace in the model the middle product of the DWC. The purity required to the middle product of the DWC has also to be required to the

stream resulting from the mixing of *B2* and *D3*. Due to the non-linear distillation behaviour, especially when high purities are required, to obtain two streams with the required B purity is easier than to obtain one stream more pure than required and the other stream less pure than required. Consequently, the purity required to the middle product of the DWC will be used as specification for B composition of both, *B2* and *D3*.

The mixture nature, the feed composition and heat condition, and the required purity of the three products define the separation problem. The steps of the proposed design methodology are:

1. Determination of α and β
2. Simulation of the prefractionator
 - shortcut calculation
 - rigorous simulation
3. Simulation of the two simple columns COL2 and COL3
 - shortcut calculation
4. Rigorous simulation of the entire Petlyuk Column
5. Change of α and β parameters values and go to 2.

The first step, the determination of α and β parameters, can be guided by the results of Fidkowski et al. (1986). Their optimal β values are proposed as initial guesses. On the other hand, an upper limit of α is known. Since practically all A in *B1* will finish at the sidestream product, specified B purity at the sidestream limits the α values.

For the simulation of the prefractionator in the second step (shortcut and rigorous simulations), the prefractionator is considered a stand-alone column with condenser and reboiler. For the shortcut calculation of the prefractionator, the values of α and β parameters are imposed as specifications. Through shortcut equations, the number of trays and the feed tray to meet the specifications and minimise distillation cost are determined.

The prefractionator is rigorously simulated with the design given by the shortcut equations. The specifications over α and β are kept. Since the new calculated operation is more accurate than the one given by the shortcut calculations, it permits easier convergence in the numerical calculation for the rigorous DWC simulation.

The third step is the shortcut calculation of the two simple columns COL2 and COL3. Also in this case, for the shortcut calculations, the columns have been considered stand-alone columns with condenser and reboiler. The prefractionator distillate calculated rigorously is the feed of COL2 and the bottom product of the prefractionator calculated rigorously is the feed of COL3.

The specifications for the shortcut calculations are the final product purity requirements. Reflux ratios, numbers of trays and feed trays for each column are given by the shortcut equations.

Finally, the rigorous simulation of the DWC is done. The specifications in this case are the purity of the three products. The design considered is given by the shortcut equations in the following way: the number of trays of the main column is the sum of the trays of COL2 and COL3. The sidestream tray corresponds to the bottom tray of COL2. The flowrates and the compositions of the connection streams from the main column to the prefractionator for the rigorous simulation are initialised with values from the COL2 and COL3 shortcuts.

The last step is the change of α and β specified values. Different α and β pairs are specified for the search of the DWC optimal design. The reboiler duty of the obtained distillations is plot in α - β plane. With enough points, the localisation of the minimum can be done.

To illustrate the design methodology, two examples are presented. Simulations have been done with the commercial simulation program ProII (PROII, 1994).

The first example is the separation of benzene, toluene and orto-xylene into 0.99 molar pure products. Feed rate is 60 kmol/hr of saturated liquid. Pressure is assumed constant at 1 atm. The thermodynamic model is SRK with binary interactions. For this mixture, assuming $\alpha=(4.65:2.15:1)$, which is a rude approximation, $\beta_P=0.315$ and $\beta_R=0.589$. In Figure 2.21, the reboiler duty for the different designs is plot.

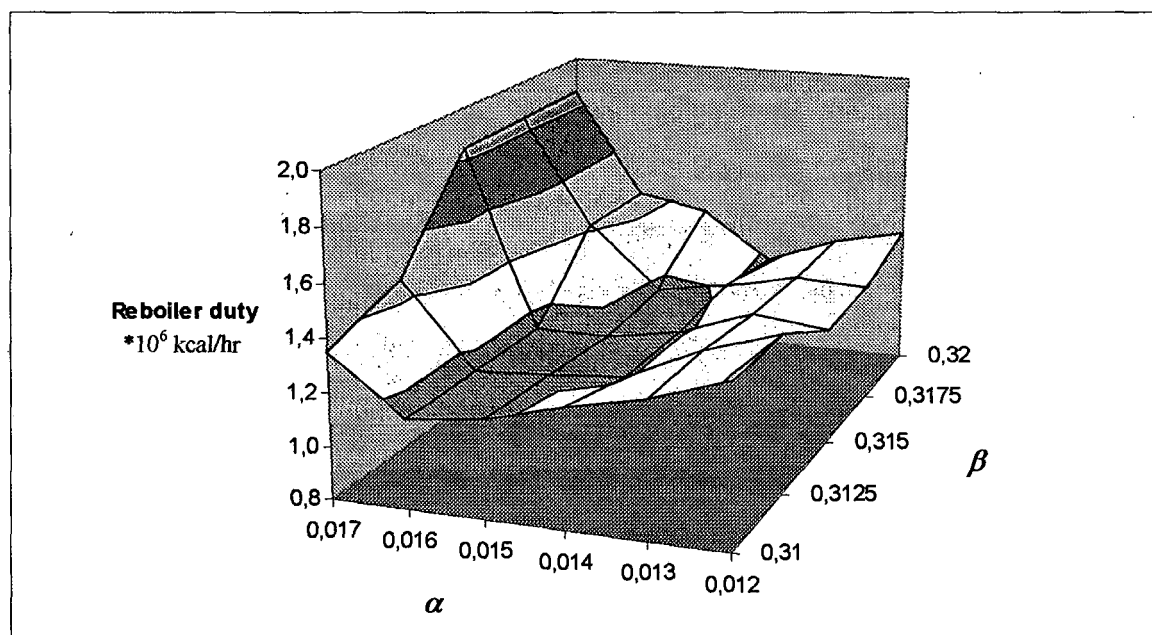


Figure 2.21: Reboiler duty for designs for the separation of a BTX mixture

It is found that the design methodology gives fewer trays to the optimal designs. This confirms that a trade-off is done between investment and energy costs. The best design that has been found has 10 trays in the prefractionator and 35 trays in the main column. The heat requirement is $1.13 \cdot 10^6$ kcal/hr, or $0.02 \cdot 10^6$ kcal for kmol of feed. Optimal α is 0.016, and optimal β is 0.315, equal to β_P .

In Figure 2.22, the reboiler duty of different designs for the separation of ethanol, propanol and butanol mixture into 0.99 molar pure products is plot. Feed rate is 60 kmol/hr of saturated liquid. Pressure is assumed constant at 1 atm. The thermodynamic model is NRTL. Assuming $\alpha=(4:2:1)$, $\beta_P=0.333$ and $\beta_R=0.575$.

The best design that has been found has a prefractionator of 11 trays and a main column of 44 trays. The heat requirement is $1.14 \cdot 10^6$ kcal/hr, or $0.019 \cdot 10^6$ kcal for kmol of feed. Optimal $\alpha=0.01$ and optimal $\beta=0.328$, very close to β_P .

In accordance with the results of Fidkowski et al. (1986), in both examples, a region with minimum boilup has been found. Interestingly, in this region, α is almost constant. Also, in accordance to the work of Annakou et al. (1996), in both examples, the optimum value of β has been found close to β_P , and not close to β_R .

The proposed design method has the advantages of using an optimisation variable (β) for which some information is known before starting the procedure, and that it can be developed using rigorous simulations of any degree of accuracy.

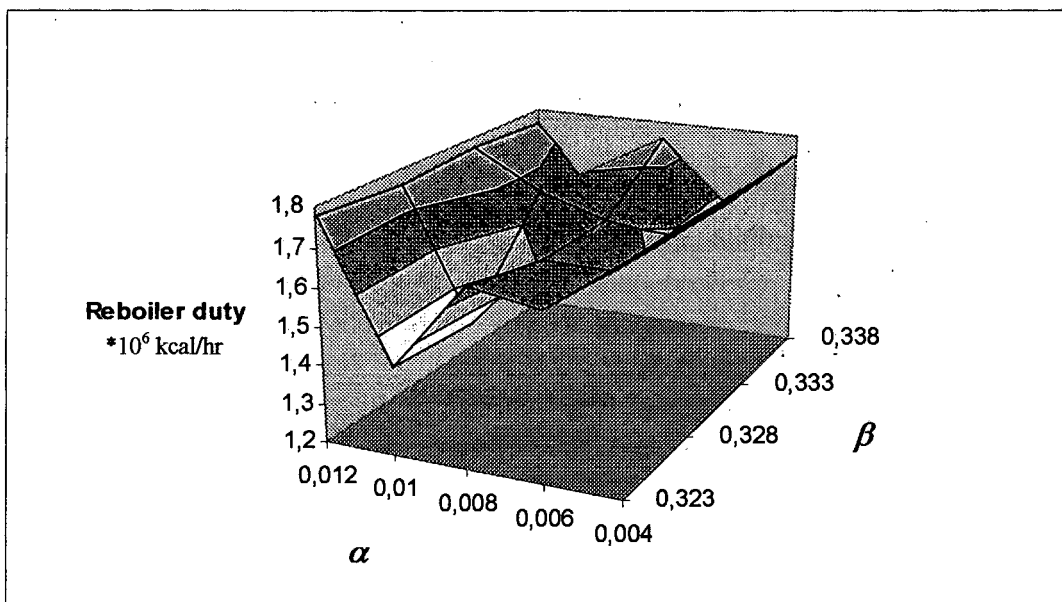


Figure 2.22: Reboiler duty for designs for the separation of an alcohol mixture

2.6.2 Design procedure with three decision variables

In this section, another heuristic method to optimise the DWC design is proposed. The method considers as design decision variables the recoveries of the three components at the DWC prefractionator. The objective is to make a greater profit of the design DOF to avoid excluding possible optimum designs in the search. Only two design variables were considered by the heuristic methods described previously. Contrarily, three design variables are considered by the methodology proposed in this section.

During the design of a DWC, the main design decision is the determination of the separation to be carried out by the prefractionator. The separation not carried out by the prefractionator will be certainly carried out by the upper and lower parts of the main column. The separation at the prefractionator can be specified at two different levels. One possibility is to determine the separation through just two decision variables (recoveries) and to assume that the rest of variables will be determined by the economic optimisation of the prefractionator system. This economic optimisation may be performed by shortcut calculations. Following this line, the work of Annakou et al. (1996) and the methodology proposed in section 2.6.1 gave special importance to the recovery of the middle component, while the work of Triantafyllou et al. (1992) gave special importance to the recoveries of the lightest and the heaviest components. On the contrary, another possibility is to determine the separation in the DWC prefractionator through the recoveries of the three components, and use them as free variables during the search of DWC optimal design. Carlberg et al. (1989) already indicated the necessity of analysing the entire range of the middle component split in the prefractionator, once the splits of the key components were specified, in order to find DWC optimum.

Shortcut methods are useful tools for preliminary design of simple distillation columns. However, there are two main reasons against the use of shortcut equations for the calculation of the DWC prefractionator design. First of all, the prefractionator cost minimisation does not implicate the whole DWC cost minimisation. Secondly, many shortcut equations for design calculations have limitations when facing multicomponent systems. For instance, the shortcut equations implemented in ProII (PROII, 1994), solve distillation columns in base to the required recovery of just the key components and therefore, they are able to find the optimal design only for specifications on the key components. Proves this the fact that, specifying A and C recoveries in a simple column, the program gives the B recovery and the number of trays of the two sections. If the obtained B recovery and the initial A recovery were specified, the same C recovery initially specified was obtained and also the same number of trays in both sections.

According to Underwood equations for minimum reflux (King, 1981), in a two section column, the recoveries of two components are specified, while the remaining recoveries and the minimum vapour rate are calculated. The reason is that in infinite columns (fixed design), only two recoveries can be specified. However, at the design stage, design may be changed in order

to specify other recoveries. Therefore, using Underwood equations, some of the DOF typical from multicomponent systems are lost. In the prefractionator of a DWC for instance, if the recoveries of A and C are specified, the recovery of the middle component becomes a dependent variable.

In order to maintain the DOF associated to the recovery of the middle component, the above mentioned limitations associated to some shortcut correlation should be overcome. The objective of the proposed design methodology is to make the middle component recovery independent considering design changes. Specifically, the feed tray location is used to determine different middle component recoveries. The importance of all three prefractionator recoveries over the global economic performance of the DWC is emphasised.

To face the design of the DWC, the simplified model shown in Figure 2.20 is used as basic structure. In relation to it, some comments are worthy. First of all, as explained in section 2.6.1, the purity required to the middle product of the DWC will be used as specification for B composition of both, $B2$ and $D3$. On the other hand, in order to avoid situations where $D1$ and $B1$ carry too much residual component (C or A, respectively) to satisfy middle product purity, lower limits on the A and C recoveries in the prefractionator will be imposed.

It has been observed that in the prefractionator, with the recoveries of A and C fixed, when the feed tray location approaches to the top, the recovery of B increases in $B1$ and decreases in $D1$. On the contrary, when the feed tray location of the prefractionator approaches to the bottom, the recovery of B increases in $D1$ and decreases in $B1$. With the recoveries of A and C fixed in the prefractionator, the change of the B split in the prefractionator causes an increase of the energy requirement in the column receiving more B and a decrease of the energy requirement in the column receiving less B. This happens as long as the B flowrate entering the column receiving less B is not too small compared to the residual component flowrate entering this column.

According to these considerations, and assuming that the separation problem is defined by the mixture nature, the feed composition and heat condition, and the required purity of the three products, the following method to optimise the design of a DWC is proposed.

2.6.2.1 The steps of the design method

This method can be summarised as follows:

- 1 - Decision of the recoveries of components A and C in the prefractionator. They must be larger than the limits imposed to them in order that the purity required to $B2$ and $D3$ can be satisfied.
- 2 - Shortcut design calculation of the prefractionator, specifying the recoveries of A and C.
- 3 - Rigorous tray by tray simulation of the prefractionator, specifying the recoveries of A and C, based on the shortcut design results.

- 4 - Shortcut simulations of COL2 and COL3. Feed streams equal to the output streams given by the rigorous simulation of the prefractionator.
- 5 - Rigorous simulation of COL2 and COL3. Design given by the shortcut design results. Adjustment of the feed tray if necessary.
- 6 - Rigorous simulation of the Petlyuk Column.
- 7 - Change of the prefractionator feed tray in the direction that minimises the larger boilup between the COL2 boilup and the COL3 boilup.
- 8 - Repetition of steps 3 to 7 until the boilups required by COL2 and COL3 are equal (if total energy does not increase).
- 9 - Change the recoveries of A and C.
- 10- Repetition of steps 1 to 9 until the optimal design is found.

In step 7, by changing the feed tray location, the recovery of B in the prefractionator is controlled. By minimising the larger vapour flow at the connection areas of COL2 and COL3, the energy requirement of the main column of the corresponding DWC will also be minimised. (Making the values of this two vapour flows closer, the most important effects of having the main column section divided in two columns is reduced).

After doing some simulations on a specific system, it is relatively easy to realise which are the main causes of the energy consumption and which are the sections charged with larger distillation effort. High A and C recoveries in the prefractionator will overload the separation effort in this part of the column whilst discharging the main column. On the other hand, as already explained, the split of B has a large influence on the distribution of the separation effort between columns COL2 and COL3. A lot of design calculation effort can be saved if the behaviour of the prefractionator is well known. This is of great help when deciding new recoveries of components A and C (step 9).

It is clear that such a heuristic method will not guarantee optimum design. However, when many simulations have been done, an idea about the goodness of the design becomes clear. In this respect, the comparison with the consumption of the conventional columns is a very valuable reference.

The shortcut calculations in the design method make it be based on minimum reflux conditions. Specifically, in each one of the three simple columns of the design model of Figure 2.20, the calculation of the number of trays is based on minimum reflux conditions. Therefore, the optimal design depends on the chosen RR/MRR values.

The design method will be used all over the work. Here as example, it has been applied to the separation of a benzene, toluene, orto-xylene mixture. 60 kmol/hr of equimolar feed have to be

separated into 0.99 molar pure products. Simulations have been done with the commercial program ProII (PROII, 1994). It is the same separation problem for which optimal design was searched through the design procedure with two specifications in section 2.6.1, and the same thermodynamic methods are used. The design found through the two specifications method had 45 trays and a boilup $V=1.134 \times 10^6$ kcal/hr. The design found by the design method proposed in this section has 46 trays and a boilup $V=0.928 \times 10^6$ kcal/hr. This is a 22% of energy savings for one more tray. The result confirms that the optimisation of the DWC with only two DOF is not complete.

2.7 Conclusions

Reversibility given by a double thermal coupling, reversibility given by the correct distribution of components into the columns, the requirement of only one condenser and reboiler, and the investment savings associated with the DWC for being constructed in only one shell are shown to make the Petlyuk Column and the DWC very attractive arrangements in terms of energy savings and cost savings. In terms of exergy however, they are less competitive because they require all the heat at the higher temperature and all the heat removal at the lower temperature. It is seen that remixing is characteristic of the DWC as well as characteristic of other distillation arrangements.

Design procedures for the Petlyuk Column and the DWC are described and analysed. The design procedures reported in the literature are found to have some limitations. Two new design procedures are proposed. One of them uses three decision variables for the optimisation. It is seen that the use of the third DOF is important to avoid excluding possible optimum designs and an example is presented to show this.