UNIVERSITAT POLITÈCNICA DE CATALUNYA

Department of Chemical Engineering

ENERGY OPTIMISATION AND CONTROLLABILITY IN COMPLEX DISTILLATION COLUMNS

Autor: Maria Serra i Prat
Director: Miquel Perrier

Barcelona, june 2000

CHAPTER 3___ APPROPRIATE ARRANGEMENTS FOR DIFFERENT

SEPARATIONS

3.1 Abstract

This chapter addresses the problem of determining which are the most economical distillation arrangements for different separations. Since many literature works address the problem, a review of the literature conclusions is done. Modelling assumptions in the different works are emphasised, and the influence of the most common assumptions on the comparisons between arrangements is analysed. Only steady state operation is considered.

With rigorous distillation models, a new contribution is added to the synthesis problem, consisting in the comparison between the DWC and the conventional column sequences. Different mixtures and different feed compositions are considered.

According to the results, the relationship between the number of DOF of the different arrangements (operation and design DOF) and their cost optimality is discussed.

3.2 Introduction

The incorporation of complex arrangements in the synthesis of distillation systems increases tremendously the complexity of the problem. Without a doubt, it is highly undesirable to synthesise and evaluate thousands of alternatives, even if efficient shortcut design methods were available. Screening rules are needed, which indicate when a complex structure has advantage over the conventional ones, and will point out the most promising alternatives.

The important number of publications indicates that a significant body of work has already been devoted to complex distillation arrangements such as the simple column with side rectifier, the simple column with side stripper, the DWC, and the Petlyuk Column. This has led to improved understanding of these arrangements and the benefits that may arise from their use. Furthermore, some works have addressed the synthesis of distillation systems comparing these complex arrangements with the conventional arrangements. However, a deficiency common to all these works can be identified. Mainly, only simple column models have been used, and this places a major question mark on the accuracy and validity of the results obtained. Until 1987 (Kaibel, 1987), finite columns were not considered. Since then, some authors have dealt with different

finite distillation arrangements, but important simplifying assumptions have still been imposed. A review of the literature conclusions is one of the objectives of this chapter.

Simplifying assumptions are useful to obtain general trends for synthesis rules. However, their consequences on the comparative results have to be analysed. This analysis is the main objective of this chapter. On the other hand, comparisons between different distillation arrangements rigorously modelled are not published. In section 3.7.1, rigorous models are used to compare the DWC with the column sequences.

As will be seen, one of the common simplifying assumptions is sharp distillation. In this work, sharp distillation indicates the separation into almost pure products. In other words, residual compositions are neglected when sharp distillation is assumed. Contrarily, for some authors, sharp distillation indicates that the two key components are adjacent in the rank order of volatility (Mc.Cabe et al., 1995).

For the valorisation of energy costs of different distillation arrangements, two main approaches are reported in the literature. In the first one, all the energy is assumed to have the same economic value. In the second one, all required amounts of energy have a temperature associated, which gives them different economic values. Specifically, the temperature required for energy exchange gives the energy a specific quality and price. This second approach is the appropriate to evaluate thermodynamic efficiency. Work of separation and exergy are the most used variables to evaluate thermodynamic efficiency.

As was early reported in the literature (Petlyuuk et al., 1965), for the same separation, some distillation arrangements may be preferable in terms of energy but other arrangements may be preferable in terms of exergy. Agrawal et al. (1998 b) stated that the range of values of feed composition and relative volatilities for which the DWC is the most thermodynamical efficient configuration is quite limited. Considering different energy levels can change the economic valorisation of a distillation arrangement. However, if different energy levels are considered, comparisons between arrangements become more complicated. To evaluate the different energy costs, available energy sources and their economic values have to be known or assumed. These parameters depend on location and time. Even more, they depend on the plant itself. Because of that, the consideration of these parameters does not give general results. On the contrary, comparison of different distillation arrangements on the basis of the required boilups (energy analysis) provides simplicity and generality. In this chapter, the difference between an energy analysis and an exergy analysis is given special importance. Because of that, the bibliography review is divided in two sections. Section 3.3 addresses comparisons between arrangements in base to the energy analysis and section 3.4 addresses comparisons between arrangements in base to the exergy analysis.

3.3 Reported results of optimal arrangements for the separation of multicomponent mixtures. Energy criterion.

In this section, in a chronological manner, works indicating the best arrangements for different separation problems are indicated, and their main results exposed. In all of these works, minimisation of the required energy is the criterion to determine the best arrangement. This energy is evaluated by the sum of the contributions of all the arrangement boilups.

Petlyuk et al. (1965) compared the direct and indirect sequences of columns with the Petlyuk Column and the DWC for the separation of an ideal ternary mixture with symmetrical properties $(\alpha=(1.2:1.1:1))$. Also some variations of the Petlyuk Column arrangement were considered. Reversible distillation was assumed, which implicates infinite number of trays as well as sharp separations. Symmetrical feed compositions $(z_A= z_C)$ with different z_B were considered, where z_i are the i molar feed compositions. For all z_B, they found that the Petlyuk Column and the DWC were the most economical of all the arrangements. Compared with the column sequences, the DWC took more advantage for large z_B. The consideration of the different Petlyuk Column variations permitted to see that the correct thermodynamic distillation sequence (property of all Petlyuk Column variations) gives advantage for large z_B. Thanks to the thermal coupling, the Petlyuk Column is advantageous also for small z_B. Optimality regions for the conventional arrangements and the arrangement shown in Figure 2.20 were defined. The non-conventional arrangement was more economical for $z_B>(1/\alpha_B)z_A$ and $z_B>(1/\alpha_B)z_C$. In the contrary case, the direct sequence was more economical than the indirect sequence if $z_A> z_C$.

Fidkowski et al. (1987) studied the optimisation of four different thermally coupled distillation systems: the simple column with side rectifier, the simple column with side stripper, the DWC and the Petlyuk Column. Infinite columns, constant relative volatilities, constant internal flowrates, and sharp distillations were considered. They found that Petlyuk Column and the DWC were thermodynamically equivalent. Optimal energy values of the column with side rectifier and the column with side stripper were the same, and larger than those of the DWC and the Petlyuk Column for all relative volatilities and feed compositions. Finally, the optimal energy values of the direct and the indirect column sequences were larger than those of the columns with side sections (and those of the DWC and Petlyuk Column) for all relative volatilities and feed compositions.

Kaibel (1987) made a comparative study with a mixture of n-hexane, n-heptane and n-octane, an almost ideal system. The DWC and the simple column with sidestream were compared. Finite columns were considered. A and C product purities were specified at 99.9%. With the same boilup and the same number of theoretical trays, the purity of the medium boiling component (heptane) increased from 83% to 99% when passing from the sidestream column to the DWC. To obtain 99% of heptane in the sidestream column, the required boilup was increased 17 times. In the work, finite number of trays and specific product purities were considered for first time.

Glinos et al. (1988) assumed infinite columns and sharp separations to compare different arrangements. Boilup values were calculated using the Underwood equations. The direct and indirect sequences were compared first. Optimality regions were found to depend on the relative volatilities, in contradiction with the work of Petlyuk et al. (1965), where the optimal regions for direct and indirect sequences did not depend on the relative volatilities. Specifically, according to Glinos et al. (1988), the optimality region for the indirect sequence (which separates B from C first) becomes small when the A-B split becomes more difficult than the B-C split. Thus, a contradiction with the common used heuristics "do the easiest split first" is also found. The authors also compared the direct and indirect sequences with the simple column with sidestream. If the sidestream purity was satisfactory, a column with sidestream above the feed was always cheaper than the indirect sequence. For an A-B split much easier than the B-C split, sidestreams with higher purity were got, but only moderate savings were possible. On the other hand, balanced volatilities resulted in more significant savings, but less pure sidestreams. A similar case occurred with a sidestream column with the sidestream below the feed tray compared to a direct sequence. A third study addressed the columns with side sections. Columns with side rectifiers and strippers were compared with the conventional sequences. The two columns with side sections had the same boilup requirement and they required less total boilup than either the direct or indirect sequences. However, savings were larger for small values of z_B and increased as both separations (A-B and B-C) became more difficult. Finally, the authors compared the Petlyuk Column with the column sequences and found that the Petlyuk Column had advantage for moderate or high z_B, specially when the A-B split was more difficult than the B-C split. The boilup savings compared to the conventional sequences were found to be more significant for the Petlyuk Column than for any other kind of complex column. When comparing all arrangements at a time, they concluded that the heuristics suggesting the use of Petlyuk Columns when most of the feed is middle component were not correct in all cases because the decision also depended on the relative volatilities. This result contradicts the result of Fidkowski et al. (1987), who said that the Petlyuk Column had lower consumption than the other complex and conventional arrangements for all relative volatilities and feed compositions.

Fidkowski et al. (1990) showed that the Petlyuk Column consumes less energy than the "Petlyuk Column" without thermal coupling for all relative volatilities and feed compositions. The assumptions of their work were the same than those made previously (Fidkowski et al., 1987).

Up to this point, despite the work of Kaibel (1987), all the works assumed infinite columns, sharp distillations, constant relative volatilites, and constant internal flows. Even with these similar assumptions, some contradictions have been found.

Trinatafyllou et al. (1990) studied finite columns. Sharp distillation assumption was removed and the influence of the required purities was studied. The influence of all component recoveries in the connection streams was studied as well. They reported only one case study, consisting in the separation of close boiling C_4. In base to the indirect sequence, the optimal DWC required 35.9% less energy.

Other arrangements are considered in the literature. For instance, Agrawal et al. (1999) analysed new simpler and easier to control alternatives to the Petlyuk Column for ternary distillations. However, other works reporting practical heuristics to classify the separation problems into optimal arrangements are not found.

3.4 Reported results of optimal arrangements for the separation of multicomponent mixtures. Exergy criterion.

Some authors have compared the different distillation arrangements in terms of exergy or work of separation criterion. In this section, in a chronological manner, works determining the best arrangements for different separation problems are indicated, and their main results exposed. In this case, minimisation of required exergy is the criterion to determine the best arrangement. Different utility costs depending on different energy temperature levels are considered in all the reported works.

Petlyuk et al. (1965) considered also the work of separation in their work. For the separation of their symmetric mixture with $z_A = z_C$, they found that the Petlyuk Column was no more the optimal arrangement for all considered values of z_B. The "Petlyuk Column" without thermal coupling required less exery than the Petlyuk Column for large z_B values. Although the Petlyuk Column was still better than the conventional sequences for all z_B, for large z_B, the differences were very small.

Doukas et al. (1978 a) studied the separation of two ternary mixtures with different A and C feed compositions. In their work, the considered arrangements were the direct and the indirect sequences, the sidestream column, the column with side stripper, and the "Petlyuk Column" without thermal coupling. The DWC was not considered. Two different energy levels were considered. The separation of a benzene, toluene, o-xylene system was studied first. Varying the amount of the lightest component (benzene) in the feed, the authors concluded that the sidestream column is the most economical of the four arrangements for low concentrations of benzene in the feed. For feed concentrations of benzene greater than 10%, the "Petlyuk Column" without thermal coupling was the most economical arrangement. Varying the amount of the heaviest component (o-xylene) in the feed, they concluded that the sidestream column was the most economical for low concentrations of o-xylene in the feed. The "Petlyuk Column" without thermal coupling was the best for higher concentrations of o-xylene. With lower relative volatilities ($\alpha = (3:2:1)$), optimal arrangements were not the same. In general, the region where the column sequences were optimal increased.

With the purpose to extend the work of Duokas et al. (1978), Alatiqi et al. (1985) studied the separation of the benzene, toluene, o-xylene mixture with varying concentrations of the intermediate component in the feed. Different required product purities were considered. The same arrangements considered in the work of Doukas et al. (1978 a) were considered. It was found that the sidestream configuration becomes less attractive compared to the column

sequences as the intermediate feed concentration becomes smaller. As conclusion they stated that columns with side strippers should be considered for separating ternary mixtures with small concentrations of the intermediate component in the feed. The range of intermediate feed compositions for which the column with side stripper is optimal increases as the purities of the products decreases (this is particulary sensitive to the purity of the intermediate product).

Tedder et al. (1978) defined the optimality regions of different distillation arrangements in the feed composition plane. Eight arrangements were considered, which included the two columns with sidestream (see Figures 2.1 and 2.2), the two column sequences, the two columns with side sections, the arrangement in Figure 2.20, and the "Petlyuk Column" without thermal coupling. The DWC was not considered. Minimum costs of all the systems were found through optimisation. Costs depending on eight different utility costs for different energy levels were considered. The optimality regions were studied separately for mixtures with different Ease of Separation Index (*ESI*). The *ESI* definition is:

$$ESI = \frac{K_A K_C}{K_B K_B} \qquad (3.1)$$

where K_i are the distribution coefficients (or K factors) of the A, B, and C components. The ratio of K factors is the relative volatility of the components. For *ESI*<1.6 mixtures, they found that, depending on the feed composition, the direct sequence, the indirect sequence, the "Petlyuk Column" without thermal coupling, the columns with side streams or the column with side rectifier could be optimal. For *ESI*>1.6 mixtures, excluding the direct sequence, depending on the feed composition, the same arrangements could be optimal. This result indicates a distribution of the optimality region that was not found comparing arrangements in base to the energy criterion.

Annakou et al. (1996) studied the Petlyuk Column exergy requirement in finite columns. They compared the Petlyuk Column with the conventional arrangements and the energy integrated conventional arrangements for the separation of several mixtures. The authors reported that, in many cases, the Petlyuk Column has considerable economic savings compared to the cheapest conventional arrangement. However it can be competitive with the heat integrated arrangements in only those few cases in what the concentration of the middle component in the feed is high and the A-B split is harder than the B-C split. This is the only work in what the DWC is compared to energy integrated conventional arrangements. Its results indicate the importance of considering the energy integration of the conventional arrangements, when it can be implemented, to properly compare different distillation arrangements.

Agrawal et al. (1998 b) proposed some equations for the calculation of the thermodynamic efficiency of the columns with side sections and the DWC. They used these equations to compare the thermodynamic efficiency of five distillation arrangements for the separation of ternary ideal mixtures into pure products. The arrangements were the direct and indirect sequences, the columns with side sections, and the DWC. The simplifying assumptions were

48

ideal mixtures, constant internal flows, no pressure drop losses. The authors found that the range of values of feed composition and relative volatilities for which the DWC was the most efficient arrangement was quite limited. They concluded that the relationship between the most efficient arrangement and the feed composition can not be correlated on the basis of *ESI* alone. For *ESI*=1, it was found that for any given composition, the most efficient choice depends on the actual values of α_A and α_B. This result is contrary to the results form Tedder et al. (1978), for which the actual values of α_A and α_B were not needed to determine the optimality regions. However, according to Agrawal et al. (1998 b), some generalisations based on *ESI* can still be made. The Petlyuk Column occupies considerable composition space as the most efficient configuration only when the value of *ESI* is in the neighbourhood of 1. When *ESI* is significantly greater than 1 (say 1.5 or higher), the configurations generally found to be the most efficient are a modified direct sequence and the simple column with side rectifier. When *ESI* is considerably less than 1 (say 0.65 or lower), the two configurations generally found to be the most efficient are a modified indirect sequence and the simple column with side stripper.

3.5 Comparison between models of finite columns and models of infinite columns

As was explained in the previous chapter, energy is the most important variable of the cost estimation in distillation processes. This fact gives practical usefulness to the results of a lot of literature works in what designs are overseen and infinite columns are assumed. However, consideration of finite columns is very important in order to be closer to real conditions. Results given for infinite columns are limited from a practical point of view. In practice, finite columns are implemented and comparisons between finite arrangements are needed.

Between the literature works reported in section 2.3, only two deal with finite columns (Kaibel, 1987), (Triantafyllou et al., 1992). In each of these works, only one case study is analysed and no general results are given. In this section, the energy requirement of different finite distillation arrangements is compared, and results are compared with the results for infinite arrangements.

The same separation used in the previous chapter to illustrate composition profiles into the different distillation arrangements has been chosen as base example in this section. It consists in the separation of a mixture with relative volatililies α=(4.65:2.15:1) into 0.99 molar pure products. Liquid saturated equimolar feed is loaded. Products are also liquid saturated streams.

In all cases, the compared energy requirements correspond to the optimal operations. In other words, the extra operation DOF are used to minimise energy consumption. Boilup units are not specified because the steady state comparisons are not influenced by the loaded feed flowrate.

3.5.1 Infinite DWC, direct sequence, and indirect sequence

According to Fidkowski et al. (1987), the optimal boilup value of a DWC at minimum reflux ratio is the one indicated in equation 3.2, where ϕ are the roots of the Underwood equation shown in 3.3, and *A*, *B*, and *C* are the A, B, and C feedflowrates.

$$V^{opt}(DWC) = \max\left\{\frac{\alpha_A * A}{\alpha_A - \phi_1}, \frac{\alpha_A * A}{\alpha_A - \phi_2} + \frac{\alpha_B * B}{\alpha_B - \phi_2}\right\} \qquad (3.2)$$

$$\frac{\alpha_A * A}{\alpha_A - \phi} + \frac{\alpha_B * B}{\alpha_B - \phi} + \frac{\alpha_C * C}{\alpha_C - \phi} = 0 \qquad (3.3)$$

The feed flowrate is not relevant for the considered model and for simplicity, A, B, and C feed flowrates are assumed to be $A=B=C=1$.

For the proposed example, $\phi_1=3.04$, $\phi_2=1.26$, and $V^{opt}(DWC)=\max\{2.89,3.79\}=3.79$.

The optimal boilup values of the direct and indirect sequences according to Fidkowski et al. (1987) can be calculated from equations 3.4 and 3.5. (The direct sequence has liquid connecting stream and the indirect sequence has vapour connecting stream).

$$V^{opt}(Direct) = \frac{\alpha_A * A}{\alpha_A - \phi_1} + \frac{\alpha_B * B + \alpha_C * C}{\alpha_B - \alpha_C} \qquad (3.4)$$

$$V^{opt}(Indirect) = \frac{\alpha_A * A}{\alpha_A - \phi_2} + \frac{\alpha_B * B}{\alpha_B - \phi_2} + \frac{(A+B)*\alpha_B}{\alpha_A - \alpha_B} \qquad (3.5)$$

For the proposed example, $V^{opt}(Direct)=5.62$ and $V^{opt}(Indirect)=5.51$.

According to these results for infinite columns, the boilup of the indirect sequence is lower than the boilup of the direct sequence, and larger than the boilup of the DWC. Specifically, $V^{opt}(Indirect)=1.45* V^{opt}(DWC)$.

3.5.2 Finite DWC, direct sequence, and indirect sequence

With finite designs, the same arrangements have been compared, for the same separation problem. Constant relative volatilities and constant internal flows are assumed in the models used for energy calculation. Other model details are described in 4.3.1.

Design methods described in the previous chapter (sections 2.4.2. and 2.6.2) have been initially used to determine the designs of the compared arrangements. A ratio of $RR/MRR=2$ has been assumed the optimal relation. The optimum DWC has 46 trays, $NM=33$, $NP=13$, $NF=7$, $NS=17$, $NCD=26$ and $NCB=8$. The optimal design for the direct train has 37 trays, $NTI=18$, $NTII=19$, $NFI=10$ and $NFII=9$. The optimal design for the indirect train has 37 trays, $NTI=18$, $NTII=19$, $NFI=9$ and $NFII=10$. Alternatively, column sequences with 46 trays have been considered. With 23 trays in each column and optimised feed trays, both the direct and the indirect sequences have $NTI=23$, $NTII=23$, $NFI=11$ and $NFII=11$.

In Table 3.1, the optimal boilups (operation optimisation) for all these distillation arrangements are shown. In the first row, there are the optimal boilups of the arrangements with optimal designs. In the second row, there are the optimal boilups of the designs with 46 trays.

50

Table 3.1: Minimum vapour flow for finite DWC and column sequences (in flowrate units)

	DWC	Direct sequence	Indirect sequence
V^{opt} with optimal designs (RR/MRR=2)	2.66 (46 trays)	3.58 (37 trays)	3.28 (37 trays)
V^{opt} with designs of 46 trays	2.66 (46 trays)	2.48 (46 trays)	2.36 (46 trays)

Looking at the results for optimal designs in Table 3.1, it is found that V^{opt}(Indirect sequnce)=1.23*V^{opt}(DWC). Comparing with the results of infinite columns, the difference in energy consumption has shortened (from 1.45 to 1.23). But more important than this are the results for columns of 46 trays. If the number of trays of the column sequences is increased until 46, these arrangements consume less energy than the DWC. Therefore, the number of trays has a large influence on the energy comparison between arrangements.

The results indicated in Table 3.1 show a case in what, with the same number of trays, the indirect sequence consumes less than the DWC. However, if more trays are added to both arrangements, keeping the same number of trays in both arrangements, the DWC consumes less than the indirect sequence. For instance, comparing a DWC and an indirect sequence with 58 trays distributed optimally through the sections, it is found that V^{opt}(Indirect sequence)=1.15* V^{opt}(DWC). This means that the ratio between the cost of the trays and the cost of the energy can make one arrangement more economic than the other or inversely. If trays were expensive in comparison to energy, columns with few trays would be optimal and the indirect sequence would be preferable. If trays were cheap in comparison to energy, columns with a lot of trays would be optimal and the DWC would be preferable.

Due to its nature, the DWC needs more trays than the sequences of columns. This is caused by the fact of having more distillation sections (Glinos et al., 1988). Normally, the number of trays needed to separate A-B and B-C in the two parts of a DWC main column is similar to the sum of the number of trays needed by the two columns of a sequence of columns. Therefore, a DWC has a number of more trays given by the number of trays in the prefractionator. Because of that, comparing arrangements with the same number of trays, the relative DWC goodness increases with the number of trays. At infinite number of trays, the DWC takes the largest advantage over the sequences of columns.

3.5.3 Infinite DWC, indirect sequence, and column with side stripper

In this section, the DWC, the column sequences, and the columns with side sections are compared. For the studied separation, the indirect sequence is better than the direct sequence and the column with side stripper is better than the column with side rectifier. Because of that, only the DWC, the indirect sequence and the column with side stripper are analysed.

According to Fidkowski et al. (1987), the minimum boilup of a column with side stripper, is the one given in equations 3.6 and 3.7.

$$V^{opt}(Stripper-Column) = \frac{\alpha_A * A}{\alpha_A - \phi_2} + \frac{\alpha_B * B}{\alpha_B - \phi_2} + V_{III}^{opt} \qquad (3.6)$$

$$V_{III}^{opt} = \frac{1}{2}\left[-\left(\frac{\alpha_A * A}{\alpha_A - \phi_2} + \frac{\alpha_B * B}{\alpha_B - \phi_2} \right) + \frac{\alpha_A * A + \alpha_B * B}{\alpha_A - \alpha_B} \right] +$$
$$+ \frac{1}{2}\sqrt{\left(\frac{\alpha_A * A}{\alpha_A - \phi_2} + \frac{\alpha_B * B}{\alpha_B - \phi_2} + \frac{\alpha_A * A + \alpha_B * B}{\alpha_A - \alpha_B} \right)^2 - 4 * \left(\frac{\alpha_A * A}{\alpha_A - \phi_2} + \frac{\alpha_B * B}{\alpha_B - \phi_2} \right) * \frac{\alpha_A * A}{\alpha_A - \alpha_B}} \qquad (3.7)$$

For the studied example, $V_{III}^{opt}=1.348$ and V^{opt}(Stripper-Column)=5.14. Therefore, at minimum reflux conditions, V^{opt}(Stripper-Column)=1.36*V^{opt}(DWC). Remember from the previous section that V^{opt}(Indirect)=1.45*V^{opt}(DWC).

3.5.4 · Finite DWC, indirect sequence, and column with side stripper

Energy consumption of the arrangements with optimal designs are compared first. Two different values of RR/MRR are considered to determine the optimal designs. They are 2 and 1.23. Results are indicated in the two first rows of Table 3.2. Optimal designs are determined following the methods described in 2.4.2, 2.4.3, and 2.6.2. Energy consumption of the arrangements with the same number of trays is compared secondly. Arrangements with 46 and 58 trays are considered. Results are indicated in the two second rows of Table 3.2.

In the following paragraphs, the designs of the compared distillation arrangements are indicated. The designs already indicated in section 3.5.2 are not indicated again.

The optimal DWC design found with RR/MRR=2 has 46 trays and the DWC design found with RR/MRR=1.23 has 58 trays. In this case, NM=40, NP=18, NF=9, NS=21, NCD=31 and NCB=10.

With RR/MRR=2, the optimal designs of the indirect sequence and the column with side stripper have 37 trays. The column with side stripper has NM=28, $NSTRIP$=9, NF=9, and NS=19. With RR/MRR=1.23, the optimal designs of the indirect sequence and the column with side stripper have 53 trays. The indirect column has NTI=26, $NTII$=27, NFI=12, and $NFII$=15. The column with side stripper has NM=38, $NSTRIP$=15, NF=12, and NS=26.

When the total number of trays has been fixed, the optimisation of the designs has been done using the remaining design DOF. With fixed total number of trays of 46, the optimal design of the column with side stripper has NM=34, $NSTRIP$=12, NF=11, and NS=23. With fixed total number of trays of 58, the indirect sequence has NTI=29, $NTII$=29, NFI=13, and $NFII$=16, and the column with side stripper has NM=42, $NSTRIP$=16, NF=13, and NS=30.

Optimal designs of the indirect sequence and the column with side stripper have fewer trays than optimal designs of the DWC. Comparing optimal designs, the DWC consumes less than these other arrangements. However, comparing designs with the same number of trays (last two rows

of Table 3.2), for total number of trays of 46, the column with side stripper is the less consuming, followed by the indirect sequence. Contrarily, for total number of trays of 58, the DWC is the less consuming, followed by the column with side stripper.

Table 3.2: Minimum vapour flow for different arrangements at different number of trays (flowrate units)

	DWC	Stripper	Indirect
V^{opt} with optimal designs (RR/MRR=2)	2.66 (46 trays)	3.12 (37 trays)	3.28 (37 trays)
V^{opt} with optimal designs (RR/MRR=1.23)	1.74 (58 trays)	1.96 (53 trays)	2.10 (53 trays)
V^{opt} with designs of 46 trays	2.66 (46 trays)	2.18 (46 trays)	2.36 (46 trays)
V^{opt} with designs of 58 trays	1.74 (58 trays)	1.87 (58 trays)	2.00 (58 trays)

To summarise the results of 3.5.3 and 3.5.4, and compare the energy consumption of the DWC with the energy consumption of the indirect sequence and the energy consumption of column with side stripper, Table 3.3 is presented, with values for infinite and finite columns.

Table 3.3: Energy consumption of DWC relative to energy consumption of indirect sequence and stripper column

	V^{opt}(Stripper-Column)/ V^{opt}(DWC)	V^{opt}(Indirect)/ V^{opt}(DWC)
Infinite columns	1.36	1.45
Optimal designs RR/MRR=2	1.17	1.23
Optimal designs RR/MRR=1.23	1.12	1.21
Designs of 46 trays	0.82	0.88
Designs of 58 trays	1.07	1.15

Comparing arrangements with the same number of trays, this number has to be large for the DWC to be preferable. The largest differences between the DWC and the other arrangements are found for infinite columns. This result is important and indicates that the DWC only develops its favourable energy properties in large columns. In accordance with that, the optimal designs of the DWC have more trays than the optimal designs of the other arrangements. However, more

important is that comparing optimal designs, the boilup of the DWC is lower than that of the other arrangements. In section 3.5.2, these conclusions were reached comparing the DWC with the sequences of columns. In this section, the same conclusions are reached including the columns with side sections in the comparisons.

Although comparisons between columns with the same number of trays have been done, they are not fully appropriate. Since there is a close relationship between the tray costs and the flowrates passing through them, in the DWC, the trays at both sides of the wall will be less expensive because flowrates in these sections are split between the two wall sides. This fact makes the medium cost of the DWC trays lower than the medium cost of the trays in other arrangements.

For proper comparisons, the optimal designs minimising energy and investment costs have to be considered. However, only energy costs can be compared. It is quite extended to consider that the optimal design corresponds to RR/MRR=1.2. However, most plants are operated at RR above the optimum because better operating flexibility is obtained (McCabe et al., 1985). In fact, the optimal RR/MRR varies with the separation problem, the distillation arrangement, and even the arrangement section. If an optimum design had the boilup of all sections 1.2 times the boilup of the infinite sections, the comparative results at finite trays would be equal to the comparative results at infinite trays.

The analysis in this section has been done for a simple model and an ordinary separation. Results are not caused by a rare behaviour specific to the studied case. Although every case will be different, the general trend found for the analysed example is expected. As conclusion of this analysis, the energy comparison between arrangements depends largely on the number of trays of the arrangements. At minimum reflux ratio, the DWC takes the largest advantage. Thus, the DWC will be a more competitive arrangement when the cost of energy has more influence than the cost of the trays.

3.6 Comparison between sharp and non-sharp distillations

Although in many works the assumptions of infinite columns and sharp (complete) separations go together, infinite columns and sharp separations are not the same assumption. For a desired purity of products, the minimum reflux occurs in an infinite column but the minimum reflux depends on the desired purity. However, the minimum reflux depends mainly on the relative volatility (McCabe et al., 1993). On the contrary, in finite columns, the reflux varies greatly depending on the products purity. In an infinite column, the energy required to obtain a product with 0.99 molar composition may be similar to the energy required to obtain a product with 0.999 molar composition, but this does not reflect real processes. On the other hand, in finite columns, total separations can not be achieved and the assumption of sharp separation is nonsense.

The assumption of sharp distillation implies that the required purity of products is not taken into account. But also, assuming sharp distillations, the recovery of some components in the

connection streams is disregarded. For instance, in a Petlyuk Column, the net quantity of C from the prefractionator top to the main column and the net quantity of A from the prefractionator bottom to the main column are not considered. Similarly, in a sequence of columns, the recovery of the residual component in the connection stream is not considered. The influence of these variables on the energy requirement is large and, as was seen in chapter two, they limit the achievable purity of products.

Alatiqi et al. (1985) showed that the relative energy consumption of different distillation arrangements depends on the purity required to the products. Despite its importance, the study of the influence of the products purity on the synthesis task is very rare.

3.7 Comparison between shortcut simulations and rigorous simulations

There is some ambiguity in the meaning of shortcut distillation. Normally, a shortcut model is understood a model in what the energy balance and the temperature are not calculated. Consequently, constant vapour flowrates are assumed through the column sections, and simple vapour-liquid equilibrium equations are used. Constant vapour rate through the column sections is a good approximation when the molar latent heats of the components are very close. Depending on the studied mixtures, simple vapour-liquid equilibrium equations may be far from representing the reality. For some systems, the assumption of constant relative volatilities may be correct, but rigorous simulations are required when the relative volatilities depend on temperature, pressure and mixture compositions.

3.7.1 Case study with rigorous simulations

In this section, some rigorous simulations are performed to compare the energy consumption of the DWC with that of the sequences of columns. Six different separation problems are studied. ProII (PROII, 1994) simulator has been used to perform the rigorous simulations.

In all the separation examples, the feed and the products are saturated liquids. Feed flowrate is 1 kmol/hr. The purities required for all product streams are 0.99 molar, the pressure drop has been neglected and the pressure into the columns is assumed at 1 atm. The thermodynamic method used for vapor-liquid equilibrium has been SRK.

Three of the separation examples correspond to separations of the benzene, toluene, o-xylene system (ESI=1). Different feed compositions distinguish the separation examples, called separation 1, 2, and 3.

- Separation 1: B largest component in feed, z_A=0.256, z_B=0.498, z_C=0.256 kmol/hr

- Separation 2: equimolar feed, z_A=0.333, z_B=0.333, z_C=0.333 kmol/hr

- Separation 3: B smallest component in feed, z_A=0.416, z_B=0.166, z_C=0.416 kmol/hr

The second three separation examples are selected to illustrate the effect of the *ESI*. The system of the first example, i-butane, n-butane, i-pentane, has *ESI*<<1 (the A-B separation more difficult than the B-C). The system of the second example, n-pentane, n-hexane, n-heptane, has *ESI* ≅1 (A-B separation as easy as B-C separation). Finally, the system of the third example, propane, i-butane, n-butane, has *ESI*>>1 (the A-B separation easier than the B-C separation). Equimolar feeds are loaded in the three separation examples, called separation 4, 5, and 6.

- Separation 4: *ESI* = 0.59, equimolar feed

- Separation 5: *ESI* = 1.04, equimolar feed

- Separation 6: *ESI* = 1.72, equimolar feed

The DWC designs have been optimised according to the method proposed in section 2.6.2, and *RR/MRR*=2. The DWC optimal designs obtained for the six separation problems are indicated in the second and third columns of Table 3.4. In the fourth column, the reboiler duties of the DWC are indicated. The fifth column reports which of the column sequences (direct or indirect) separates the mixtures with lower energy requirement, and the energy and number of trays needed. The last column indicates the percent of energy savings of DWC in comparison with the better column sequence.

Results obtained from separations 1, 2, and 3 indicate that the better use of the energy savings capacity of the DWC is made when the presence of B in the feed is larger, which is in accordance with the results in the literature. According to the results obtained from separations 4, 5, and 6, the DWC is more appropriate for those systems with *ESI* close to unity. When one of the separations is more difficult than the other, great difficulties to make equal the vapour flows at the connecting areas of COL2 and COL3 have been found (see Figure 2.20). The separation of the system with *ESI*=1.72 requires less energy in an indirect sequence than in a DWC. This result also agrees with the results in the literature (Agrawal et al., 1998).

From the second separation example, V^{opt}(Indirect)=1.25* V^{opt}(DWC). The same comparison with shortcut models gave V^{opt}(Indirect)=1.23* V^{opt}(DWC) in section 2.5. The difference is small due to the fact that the benzene, toluene, o-xylene system is quite ideal.

3.8   Number of sections and energy optimisation

In chapter two, it was seen that the number of distillation sections differs from one arrangement to another and that the number of sections is representative of the number of design DOF. According to the results in this chapter the relation between the number of sections and the energy optimality of a distillation arrangement can be analysed. In Table 3.5, the number of sections of the most relevant arrangements is indicated. The side stream column is the arrangement with fewer sections, the column sequences have the same number of sections than the columns with side sections, and the Petlyuk Column and the DWC are the arrangements with more sections.

Table 3.4: DWC energy/investment requirements compared with the corresponding distillation train

	Prefractionator	Main Column	DWC	Better Train	
Separation	Number of trays Feed tray	Number of trays Feed trays Product trays	Reboiler duty	Better train Number of trays Reboiler duty	Savings
1 ESI=1 More B	10 5	35 8,28 1,8,19,28,35	68.3e6 J/kmol	Indirect 37 $88.7*10^6$ J/kmol	22.9%
2 ESI=1 equimolar	13 7	33 8,26 1,8,17,26,33	64.5e6 J/kmol	Indirect 37 $80.8*10^6$ J/kmol	20.1%
3 ESI=1 Less B	15 8	32 8,28 1,8,17,28,32	56.1e6 J/kmol	Indirect 36 $65.6*10^6$ J/kmol	14.3%
4 ESI=0.59 equimolar	15 4	47 15,40 1,15,31,40,47	77.0e6 J/kmol	Direct 49 $96.8*10^6$ J/kmol	20.4%
5 ESI=1.04 equimolar	13 8	32 7,24 1,7,14,24,32	51.6e6 J/kmol	Direct 35 $79.3*10^6$ J/kmol	34%
6 ESI=1.72 equimolar	15 10	45 6,32 1,6,16,32,45	96.2e6 J/kmol	Indirect 46 $81.3*10^6$ J/kmol	no savings

Table 3.5: Number of sections of different distillation arrangements

Side stream column	Direct and indirect sequences	Side stripper and side rectifier	DWC - Petlyuk Column
3	4	4	6

First of all, the number of sections of one arrangement is not the only factor determining its ability to save energy. Not only the number of sections but also the way they are connected between them define an arrangement and its ability to save energy. Different arrangements with the same number of sections do not consume the same. For instance, the column sequences and the columns with side sections do not consume the same energy and they have the same number of sections, which is four.

According to the results of Fidkowski et al. (1987), the energy requirement of the DWC and the Petlyuk Columns (6 sections) is lower than the energy requirement of the columns with side sections (4 sections), which is lower than the energy requirement of the column sequences (4 sections), for all positive values of relative volatilities and feed compositions. Results apply to ideal solutions separated in almost pure components in infinite columns. In these restricted cases, the arrangement with more sections is optimal.

As was seen in section 2.5.6, one of the most influent contributions to the reversibility of a distillation column is the reversibility of the mixing at the feed tray, which can only occur if only one component is stripped out in each section. This is a characteristic of the Petlyuk Column and the DWC. To strip out only one component in each section, $n*(n-1)$ sections are required. With fewer sections, reversible mixing at the feed trays is not possible. In this sense, the number of sections and the optimality of an arrangement can be related. It is important to say however, that the savings given by the reversibility at the feed tray can be in some cases a small contribution compared to other aspects and because of that, some cases can be found where arrangements with more sections need more energy.

For separation example 6 in 3.7.1, the optimal DWC requires more energy than the optimal indirect sequence of columns. Also in the literature, it has been said that the optimality of the DWC depends on the relative volatilities of the mixture components (Glinos et al., 1988), (Agrawal et al., 1999). Therefore, the general statement "arrangements with fewer sections require more energy" is not true. For some mixtures and specified purities, arrangements with fewer sections can be more adequate.

3.9 Operational DOF and energy optimisation

In this section, the relation between the number of operational DOF and the energy optimality in different distillation arrangements is considered. In Table 3.6, the number of operation DOF of the most relevant arrangements is indicated.

The same examples exposed in the previous section show that in general, the statement "arrangements with more operational DOF require less energy" is not true. However, it is true in the restricted case of the assumptions of Fidkowski et al. (1987).

58

Table 3.6: Operational DOF of different distillation arrangements

Side stream column	Direct and indirect sequences	Side stripper and Side rectifier	DWC- Petlyuk Column
-1	1	1	2

3.10 Conclusions

In this chapter, a review of the literature works addressing the synthesis problem for ternary distillations is done. The simplifying assumptions in the models of the reported works differ but generally, their degree of accuracy is low. Comparing the results of different works, some contradictions are found. This indicates that particular assumptions can change the conclusions about the energy consumption of an arrangement relative to the others. The influence of different assumptions on the comparison between arrangements is analysed. Results are largely influenced by the assumption of minimum reflux conditions. Studying the influence of the number of trays in the different arrangements, it is found that the Petlyuk Column and the DWC require large columns in order to be advantageous. Therefore, these arrangements are more competitive when the energy cost is high compared to the trays cost.

It can also be concluded that the literature provides with enough theoretical works comparing different arrangements simply modelled. Consideration of realistic models will not provide general conclusions, but will be interesting from a practical point of view. The study of specific applications with their particular detail will be very useful. In fact, rigorous simulations will be required in each particular case to compare the performance of the different distillation arrangements.

From rigorous simulations of six different separation examples, the following has been observed:

- For a mixture with $ESI=1$ and symmetric feeds ($z_A=z_C$) separated into 0.99 moral purity products at atmospheric pressure, the DWC energy savings are larger when z_B is large.

- For different mixtures and equimolar feeds separated into 0.99 molar purity products at atmospheric pressure, the DWC energy savings are larger for ESI close to unity.