

Distillation Configurations and Their Energy Requirements

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A method for systematic generation of all possible configurations of distillation columns for multicomponent separation is described. Classic configurations with sharp splits and all the possible (partially and fully) thermally coupled systems are generated by listing all the splits between components and applying various interconnecting streams and column stacking. Separation systems with multiple streams producing the same product (with the same or different purity) are also being generated. Additionally, a method for systematic evaluation of minimum vapor flows in all the configurations has been developed. The method can be used in evaluating various possibilities to select the optimum configuration for a new design or to improve an existing plant. Energy requirements of various column configurations for separation of four components have been evaluated and compared. © 2006 American Institute of Chemical Engineers AIChE J, 52: 2098–2106, 2006

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Introduction

There are several possible column configurations for separation of ternary mixtures: direct split, indirect split, side stripper, side rectifier, system with prefractionator, fully thermally coupled system, and a column with a side stream. Then there are some additional configurations, called side rectifier with vapor connection (RV) and side stripper with liquid connection (SL). A column with a dividing wall was invented over half a century ago, but it has been "rediscovered" and built just in the last decades. Also, a so-called "more operable" fully coupled system can be used to distill a ternary mixture. These various configurations have been coming into light gradually in a somewhat chaotic, evolutionary process.

Synthesis strategies for multicomponent mixtures were described by Rathore et al.,⁵ and a quaternary example was shown. Energy integration was taken into account; however, the thermally coupled systems, or prefractionator columns, were not included.

The concept of a superstructure appeared in the 1970s. A

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superstructure contains all the possible connections between the columns, and each specific distillation configuration could be easily obtained from the superstructure by simply deleting some of its elements (streams or column sections). Once a superstructure is known, it can be used, together with a robust MINLP algorithm, to find the optimal configuration at the optimum operating point.

Sargent and Gaminibandara⁶ proposed a superstructure of distillation columns. It was initially believed to contain all the possible column configurations. After all, it did contain all the possible ternary configurations. However, Agrawal⁷ discovered that there is a quaternary column configuration (satellite system) that is not contained in this superstructure.

Superstructures are still used, especially by the researchers specializing in MINLP algorithms. Creating a good superstructure is not easy. If we provide stream connections between all the possible points of the flowsheet, we may temporarily exhaust all the possibilities. Such a superstructure is very complicated, especially since it contains a web of some nonsense and trivial connections that just overshadows the original problem and makes it unnecessarily too complicated. Filtering out some subsets of a superstructure easily leads to omissions of valid configurations.

Generating all the possible thermally coupled configurations

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for multicomponent mixtures could be a complicated task. Agrawal⁸ presented an algorithmic method of synthesizing all the possible column configurations for multicomponent distillation. The principles of the method are simple, but the details are somewhat overwhelming.

Another method to generate only thermally coupled systems was proposed by Rong et al.9 It is based on exploiting all the combinatorial possibilities of various splits between the components, including sloppy splits.

The method of generating distillation configurations that is described here is similar. However, in addition to just drawing thermally coupled configurations, other column systems are considered here and the detailed algorithm of their evaluation is provided. Furthermore, energy requirements of separation in various quaternary systems (thermally coupled configurations, configurations with liquid only interconnecting streams, and configurations with some liquid and some vapor interconnecting streams) are compared and discussed here.

Mixtures that do not form azeotropes are assumed. Energy requirements are assumed to be proportional to the minimum vapor flow. Minimum vapor flow is calculated using the Underwood method, 10 assuming constant molar overflow and constant relative volatilities of components.

Some important components of capital cost, for example, column diameter and heat exchange area, will also increase proportionately to the vapor flow.

Component Splits and Basic Configurations

Let us consider a non-azeotropic mixture of components A, B, C, D, E, . . . where components are listed in decreasing order of volatilities. A split is defined as the action of separating a mixture into two products that can be pure components or mixtures. Therefore, all the possible splits are determined by possible products of separation.

For example, A/BC denotes the split of feed mixture ABC into the more volatile component A and the less volatile mixture BC. This is an example of a so-called sharp split, where each component appears in only one of the products.

Split ABC/CD is the split of mixture ABCD into the more volatile mixture ABC and the less volatile mixture CD. This is a non-sharp or sloppy split, where component C distributes between the top and the bottom product.

Let us assume that the distillate does not contain the heaviest component and the bottom product does not contain the most volatile component.

Each split corresponds to a simple (basic) distillation column with one feed and two products. These splits may also be represented on the state task network. There is no assumption about the thermodynamic states of the feed and the products, nor about the type of reboiler or condenser. For example, one may use a total condenser, a partial condenser, or no condenser at all, where reflux is provided from an outside source as in a thermally coupled system.

Table 1. Possible Products of Separation of Ternary Mixture ABC

| Distillate | Possible Bott | tom Products |
|------------|------------------|--------------|
| A AB | (1) BC (2) BC | (3) C |

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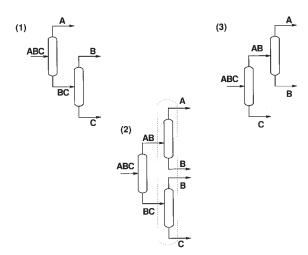


Figure 1. Basic configurations for separation of ternary mixtures.

(1) Direct split, (2) transition split, (3) indirect split.

Selected combinations of splits determine a basic configuration of columns—a skeleton of the real column configuration, where types of interconnecting streams and column stacking are not yet defined. Examples of basic column configurations are given below for ternary, quaternary, and five component mixtures.

Ternary mixture

Possible products of the separation of a ternary mixture ABC are shown in Table 1. They correspond to the three known splits: (1) A/BC (A in distillate, BC in the bottoms), (2) AB/BC (AB in distillate, BC in the bottoms), and (3) AB/C (AB in distillate, C in the bottoms). These splits define all basic configurations of columns for ternary separation, shown in Figure 1. Product columns A/B and B/C in the second basic configuration can be joined together, because they have the same component: component B as the bottom and the top product, respectively. The possibility of joining these columns is shown in Figure 1 by a dotted line encompassing columns A/B and B/C. The splits are also known as a direct split (1), a transition split (2), and an indirect split (3). A transition split is actually the optimal AB/BC split, where component B distributes between the top and bottom product in the ratio that minimizes total energy of this separation.

Quaternary mixture

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Possible products of separation of quaternary mixture ABCD are shown in Table 2.

There are six possible splits in a quaternary column: (1) A/BCD, (2) AB/BCD, (3) AB/CD, (4)ABC/BCD, (5) ABC/ CD, and (6) ABC/D.

Table 2. Possible Products of Separation of Quaternary **Mixture ABCD**

| Distillate | Possible Bottom Products | | | | |
|------------|--------------------------|--------|-------|--|--|
| A | (1) BCD | | | | |
| AB | (2) BCD | (3) CD | | | |
| ABC | (4) BCD | (5) CD | (6) D | | |

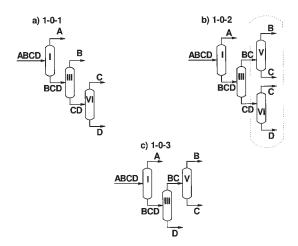


Figure 2. Basic configurations 1-0-1, 1-0-2, and 1-0-3 for separation of quaternary mixtures.

The ternary mixtures resulting from these splits may be separated in one of the three possible basic configurations, as described above.

We will name the resulting configurations using three digits: The first digit is the number of the split for the quaternary mixture (1-6), the second digit is the split number used to separate the distillate from the quaternary column (0 if the mixture contains less than three components and 1, 2, or 3 for the ternary mixture), and similarly, the third digit describes the kind of split used to separate the bottom product.

In quaternary split (1) (A/BCD) there is no need to separate the distillate; the bottom product, mixture BCD, can be separated in three ways (using direct split, transition split, or indirect split). This gives column configurations 1–0-1, 1–0-2, and 1-0-3, shown in Figure 2. These configurations are also named as a, b, and c for greater convenience in referring to them.

Similarly, there are three possible column configurations for a quaternary split (2) AB/BCD: 2-0-1, 2-0-2, and 2-0-3 (configurations d, e, and f, in Figure 3).

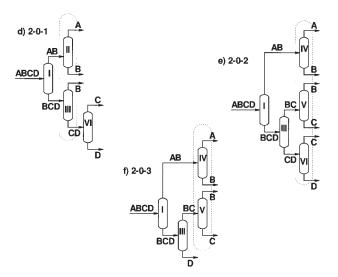


Figure 3. Basic configurations 2-0-1, 2-0-2, and 2-0-3 for separation of quaternary mixtures.

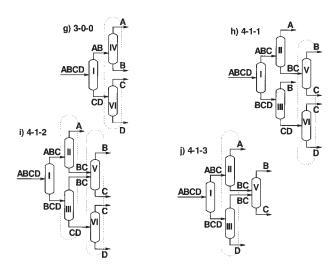


Figure 4. Basic configurations 3-0-0, 4-1-1, 4-1-2, and 4-1-3 for separation of quaternary mixtures.

For split (3) (AB/CD) there is only one possible combination of columns: 3-0-0 (or g), shown in Figure 4.

For split (4) (ABC/BCD) there are nine possible column configurations, shown in Figures 4-6. These are all possible combinations of three ternary splits for the distillate (ABC) and three splits of the bottoms (BCD). Interestingly, in four of these cases, the same component is produced from different parts of the flowsheet. In case 4-1-1, component B is produced from two different columns as a distillate. In case 4-3-3, component C is produced from two different columns as a bottom product. Also, note that in case 4–2-1, component B is produced from two different places in the flowsheet in distillates and from a third place as the bottom product. Similarly, in case 4-3-2, component C is produced from three different columns.

Configuration 4–2-2 in Figure 51 is the base configuration for the fully thermally coupled system. Three possible configurations for split (5) (ABC/CD) are shown in Figure 7, and three configurations for split 6 are given in Figure 8.

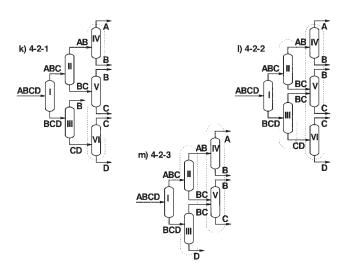


Figure 5. Basic configurations 4-2-1, 4-2-2, and 4-2-3 for separation of quaternary mixtures.

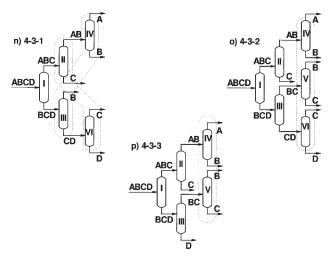


Figure 6. Basic configurations 4–3-1, 4–3-2, and 4–3-3 for separation of quaternary mixtures.

Total number of basic configurations for quaternary separation is 22.

Five-component mixture

Ten possible splits for a five-component mixture are listed in Table 3. As a result of each split, we may obtain pure components and/or binary, ternary, or quaternary mixtures. These mixtures can be further separated in various alternative configurations, depending on the type of split used. As described above, there are 3 possible basic column configurations for separation of a ternary mixture and 22 basic configurations to separate four components. Therefore, the total number of distillation configurations can be calculated as follows in Table 4. There are 719 basic column configurations for separation of a five-component mixture. This number includes also the configurations where one product is made from multiple places in the system.

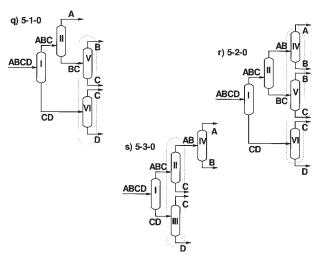


Figure 7. Basic configurations 5–1-0, 5–2-0, and 5–3-0 for separation of quaternary mixtures.

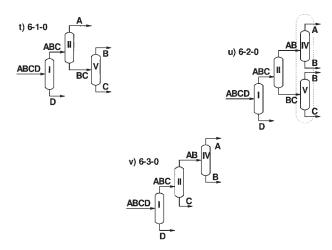


Figure 8. Basic configurations 6-1-0, 6-2-0, and 6-3-0 for separation of quaternary mixtures.

Interconnecting Streams

The streams connecting the columns may have various thermodynamic states. Examples of such streams leaving a given column (see Figure 9) are:

- (1) liquid
- (2) vapor
- (3) liquid and vapor of the same compositions, fed to different locations (liquid above vapor),
- (4) a two-phase stream or two separate streams of liquid and vapor in equilibrium fed to the same location
 - (5) a two-phase stream and
- (a) in case of a bottom product—a liquid stream fed above the two-phase stream;
- (b) in case of the top product, there will be a two phase stream and a vapor stream fed below it.

Furthermore, in thermally coupled systems, there is also a liquid or vapor stream going in the direction opposite to the streams listed above. This returning stream forms or supplements reflux or boilup in the given column. It creates 5 additional possible combinations for the top product and 5 combinations for the bottom product transferred to a next column (Figure 10). Altogether there are 10 possible types of each interconnecting stream. More possibilities for the interconnecting streams can be thought of, but these 10 are probably the simplest types of interconnecting streams.

Basic configuration (1) for a ternary mixture (direct split) has one interconnecting stream, so there can be ten column configurations corresponding to basic configuration (1). There are also ten configurations corresponding to basic configuration (3). There are two interconnecting streams in basic configuration (2), so there are $10^2 = 100$ possible corresponding configurations.

Table 3. Possible Products of Separation of Five-Component Mixture ABCDE

| Distillate | Possible Bottom Products | | | | |
|------------------------|--|-------------------------------|------------------|--------|--|
| A AB ABC ABCD | (1) BCDE (2) BCDE (4) BCDE (7) BCDE | (3) CDE (5) CDE (8) CDE | (6) DE (9) DE | (10) E | |

Table 4. Number of Basic Configurations for Separation of Five-Component Mixture

| Split | Distillate/Bottoms | Number of Configurations |
|-------|--------------------|--------------------------|
| 1 | A/BCDE | 22 |
| 2 | AB/BCDE | 22 |
| 3 | AB/CDE | 3 |
| 4 | ABC/BCDE | 3*22 |
| 5 | ABC/CDE | 3*3 |
| 6 | ABC/DE | 3 |
| 7 | ABCD/BCDE | 22*22 |
| 8 | ABCD/CDE | 22*3 |
| 9 | ABCD/DE | 22 |
| 10 | ABCD/E | 22 |
| Total | | 719 |

The total number of all quaternary configurations is 377,500, as shown in Table 5.

Column Stacking

We assume that all the basic columns operate at a similar pressure, and heat integration of columns due to different pressures is not considered. However, heat integration of columns due to different compositions (and resulting temperatures) may be desired.

Some basic columns can be connected vertically, one on top of the other, or simply lumped into one column. It is possible in a case where the same product appears in two different streams: as a top product of the lower column and as the bottom product of the upper column.

This connection allows liquid and vapor to flow vertically between the two basic columns. The diameter of the column containing two basic columns (that now become column sections) may be constant or it may be different for both sections. Column stacking enables us to re-utilize energy and to save capital.

If there is no heat exchanger between the two stacked columns, and minimum vapor flows in these columns are different (which is usually the case), then only one of the sections operates close to the minimum vapor flow and the other section must be above its minimum vapor flow. Therefore, the diam-

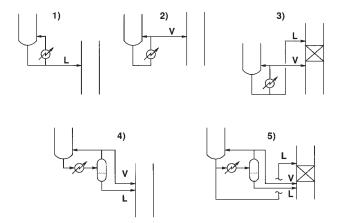


Figure 9. Possible kinds of interconnecting streams.

(1) Liquid; (2) vapor; (3) liquid and vapor of the same compositions, fed to different locations (liquid above vapor); (4) a two-phase stream or two separate streams of liquid and vapor in equilibrium fed to the same location; (5) a two-phase stream and (in case of a bottom product) a liquid stream fed above the two-phase stream.

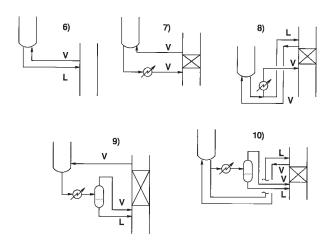


Figure 10. Various kinds of interconnecting streams for thermally linked column (cases 6-10 correspond to cases 1-5 from Figure 9).

There is an additional vapor stream (for the bottom product connection) or a liquid stream (for the top product connection, not shown) flowing in the opposite direction.

eter of the section operating above minimum reflux may be much bigger than necessary. That may increase the capital cost of that section, on the one hand, but on the other hand, it may be cost effective when the diameter of the entire stacked column is unchanged. In these cases the capital cost must be considered in addition to the energy cost.

The first possibility of column stacking is shown for the transition split of a ternary mixture—Figure 1, configuration 2, where column AB is placed on top of column BC. The stacking is possible because the same product B is made from the

Table 5. Total Number of Possible Quaternary Configurations with Various Interconnecting Streams

| Basic Configuration | Number of Interconnecting Streams | Number of Possible Configurations |
|---------------------|---|---|
| 1-0-1 | 2 | 10^{2} |
| 1-0-2 | 3 | 10^{3} |
| 1-0-3 | 3 2 3 | 10^{2} |
| 2-0-1 | 3 | 10^{3} |
| 2-0-2 | 4 | 10^{4} |
| 2-0-3 | 3 | 10^{3} |
| 3-0-0 | 2 | 10^{2} |
| 4-1-1 | 4 | 10^{4} |
| 4-1-2 | 4 | 10^{4} |
| 4-1-3 | 3 | 10^{3} |
| 4-2-1 | 5 | 10 ⁵ |
| 4-2-2 | 5 | 10 ⁵ |
| 4-2-3 | 4 | 10^{4} |
| 4-3-1 | 4 | 10^{4} |
| 4-3-2 | 5 | 10 ⁵ |
| 4-3-3 | 4 | 10^{4} |
| 5-1-0 | 3 | 10^{3} |
| 5-2-0 | 4 | 10^{4} |
| 5-3-0 | 3 | 10^{3} |
| 6-1-0 | 2 3 | 10^{2} |
| 6-2-0 | | 10^{3} |
| 6-3-0 | 2 | 10^{2} |
| | | $3*10^5 + 7*10^4 + 7*10^3 + 5*10^2$ |
| Total | | = 377,500 |

Table 6. LV Systems with the Minimum Vapor Flow Within 10% from the Optimal Configuration

| Split | A-Rich Mixture | B-Rich Mixture | C-Rich Mixture | D-Rich Mixture | M Mixture |
|-------|----------------|----------------|-------------------|----------------|---------------|
| Бри | A-Rich Mixture | B-Rien whature | iviixture | D-Rich Whature | WIWIXTUIC |
| eee | ALL-(act) | defklmnop | ilogrs | ALL-(vt) | eilor |
| eed | ALL-(abcdnst) | ALL-(abcqstuv) | ALL | ALL | ALL-(t) |
| ede | ALL-(cfjmptuv) | ALL-(qt) | behiklrnogs | behiklnors | ALL-(acfjqtv) |
| dee | ALL | defklmnop | hiklqr | efghijklmopr | ALL-(abcqtuv) |
| edd | beilors | ALL-(acjqtv) | beilogrs | ALL-(t) | beilors |
| ded | ALL | defklmnop | ALL-(abcdftv) | ALL | efghijklmopqr |
| dde | ALL-(c) | defklmru | behiklnogrs | deklmr | deklmru |
| ddd | ALL-(ac) | deflm | ilqrs | ALL-(vt) | 1 |

Listed configurations are denoted by letters as in Figures 2-8. ALL means all configurations.

bottom of basic column AB and from the top of column BC. The columns to be stacked are marked in Figure 1 (and in subsequent figures) by a dotted line around them.

Usually, energy requirements to separate these two pairs of components are different and minimum vapor flows in the basic columns are different. The stacking may be realized in two ways:

- One way is to make both columns operate at the higher vapor flow; then one of the basic columns will operate at minimum reflux conditions and the other one above the minimum reflux (of course, operation at minimum reflux would require an infinite number of stages in the column; it is assumed here just for the sake of the minimum vapor flow calculations).
- Another way is to place a heat exchanger between the two stacked columns and operate both stacked basic columns at minimum reflux. The heat exchanger could be either a reboiler or a condenser, depending on which vapor flow controls. For example, if the minimum vapor flow in the bottom column BC is smaller than in AB, then a reboiler is needed between these two columns, to generate additional vapor for A/B separation. In the present approach we will assume that all the basic columns operate at minimum reflux and the necessary heat exchangers between the basic columns are in place.

Stacking based on the principle that the same product is made from the bottom of one column and from the top of another column is shown for the following quaternary configurations: b, d, e, f, h, i, j, k, l, m, n, o, p, q, r, s, and u (Figures 2–8). Interestingly, in cases i, j, l, and m, the common product is not a pure component but a mixture BC. This may give rise to some additional questions about optimal compositions of both products BC. For the fully coupled quaternary configurations, it has been found that transition splits always provide minimum energy requirements. For other configurations it has not been proven yet, and BC composition may need to be optimized.

An interesting case of stacking is shown for configuration n (4–3-1, Figure 6), where binary columns are combined with columns separating ternary mixtures. The resulting configuration is the well-known satellite system.⁷

Configurations where the same product is made from multiple locations provide more than one option of stacking. For example, in configuration k (4–2-1, Figure 5), column AB can be stacked on top of column BCD or on top of column BC or both. This last solution may provide some new technical challenges. Similarly, in configuration o (4–3-2, Figure 6), column CD can be situated below column BC or column ABC, or it can be combined with both these columns. In the present work, these alternative ways of stacking were not considered, that is,

in both systems k and o, only binary columns (AB, BC, and CD) are stacked to form one column.

The other possibility of stacking the columns appears when distillate of the lower column boils at higher temperature than the bottoms of the upper column. The pressures of the columns are similar; hence, the temperatures are determined by compositions only. Examples include stacking columns: AB and CD in configurations d, g, and s; AB and BCD in e and f; and ABC and CD in q and r. Stacking of the columns with different product compositions requires additional equipment to prevent mixing of different products. This additional equipment may be:

- New column section between the stacked columns, to change composition upward, from higher boiling mixture to the lower boiling mixture
- Heat exchanger that would allow passing heat from the lower column to the upper column but it would keep material streams separated.

In almost all the examples above, this kind of stacking prevents stacking the columns with the same product. Therefore, this kind of stacking will not be used here. The only exception is configuration g, where a heat exchanger between columns AB and CD is assumed.

Procedure for Calculating Minimum Vapor Flow

Minimum vapor flow is calculated using the Underwood method.¹⁰

Detailed calculations depend on types of component splits in a given column. These include sharp splits, where components appear only in the top or in the bottom product, and splits with distributing components (sloppy splits), where certain components are contained in both products. For each split one can derive formulas to calculate the minimum vapor flow and the distillate flow rate for each component. For sloppy splits the split of

Table 7. The Ratio of Minimum Vapor Flows of the Highest and the Lowest Energy Consuming Configurations in LV Systems

| Split | A-Rich Mixture | B-Rich Mixture | C-Rich Mixture | D-Rich Mixture | M Mixture |
|-------|-------------------|-------------------|-------------------|-------------------|--------------|
| eee | 1.14 | 2.12 | 1.51 | 1.23 | 1.76 |
| eed | 1.24 | 1.95 | 1.08 | 1.02 | 1.14 |
| ede | 1.25 | 1.20 | 1.22 | 1.30 | 1.21 |
| dee | 1.02 | 1.28 | 2.20 | 1.38 | 1.19 |
| edd | 1.49 | 1.63 | 1.91 | 1.12 | 1.83 |
| ded | 1.07 | 1.38 | 1.18 | 1.09 | 1.83 |
| dde | 1.13 | 2.01 | 1.69 | 1.77 | 1.86 |
| ddd | 1.16 | 2.42 | 2.30 | 1.17 | 2.20 |

Table 8. L Configurations with the Minimum Vapor Flow Within 10% from the Optimal L Configuration

| Split | A-Rich Mixture | B-Rich Mixture | C-Rich Mixture | D-Rich Mixture | M Mixture |
|-------|-------------------|-------------------|-------------------|-------------------|---------------|
| eee | abc | d | iloqrs | fgjmtu | el |
| eed | abcejg | degkn | ALL | ALL | ALL-(tv) |
| ede | abc | adghkn | behiklnoqrs | beilogrsu | ALL-(cptuv) |
| dee | abchijq | defklm | lr | egjlr | ALL-(copstuv) |
| edd | b | adghkn | beilogrs | cfjmptuv | beilogrs |
| ded | abcegijt | eklm | egijklmnoqrs | ALL-(abhpq) | egjlr |
| dde | abc | def | gnops | lmru | defklmru |
| ddd | abc | d | ils | tuv | 1 |

Listed configurations are denoted by letters as in Figures 2–8. ALL means all configurations.

distributing components is optimized to give the minimum value of the minimum vapor flow in the given column (transition split). This leads to the total minimum of the minimum vapor flow for the fully thermally coupled system of columns.11 It is assumed here (but not proven) that transition splits will also give total minimum vapor flow for other configurations.

Calculations of minimum vapor flow are performed for each distillation column, beginning with the column separating quaternary mixture ABCD (column I), then continuing for ternary columns separating ABC (column II) and BCD (column III), and ending on binary columns AB, BC, and CD (columns IV, V, and VI). Column numbering is also shown in Figures 2–8. If a given sequence does not contain one of the columns, then corresponding calculations should be omitted.

The detailed algorithm for a quaternary mixture is described below. It can easily be extended to mixtures containing more than four components:

- (1) Flow rates of components in the feed and feed compositions are calculated.
- (2) Feed quality q is calculated. Thermodynamic state of the quaternary feed is given (for example, q = 1 for boiling liquid). The value of q for the next columns depends on the type of interconnecting stream, that is, 0 for vapor, 1 for liquid. For the thermally coupled connection, the value of q is calculated as the ratio of the liquid feed to the total "net" feed. The resulting q may be positive or negative, depending on the direction of the streams. For simplicity, no other types of interconnecting streams were considered.
 - (3) The roots of the Underwood equation are calculated.
- (4) The minimum vapor flow in the rectifying section and component distillate flow rates are calculated. Also, distillate flow is determined by summing up the flow rates of components that appear in the distillate.
- (5) Component flow rates in the bottoms are calculated from material balance.

Table 9. The Ratio of Minimum Vapor Flow of the Worst to the Best L Configuration

| A-Rich Mixture | B-Rich Mixture | C-Rich Mixture | D-Rich Mixture | M Mixture |
|-------------------|---|---|--|---|
| 2.21 | 2.03 | 1.57 | 1.30 | 2.06 |
| 1.78 | 1.71 | 1.09 | 1.08 | 1.15 |
| 1.79 | 1.20 | 1.21 | 1.32 | 1.19 |
| 1.24 | 1.27 | 2.06 | 1.54 | 1.22 |
| 1.92 | 1.55 | 1.89 | 1.41 | 1.49 |
| 1.24 | 1.37 | 1.19 | 1.15 | 1.88 |
| 1.54 | 1.97 | 1.51 | 1.66 | 1.50 |
| 1.75 | 2.18 | 2.09 | 1.64 | 1.94 |
| | Mixture 2.21 1.78 1.79 1.24 1.92 1.24 1.54 | Mixture Mixture 2.21 2.03 1.78 1.71 1.79 1.20 1.24 1.27 1.92 1.55 1.24 1.37 1.54 1.97 | Mixture Mixture Mixture 2.21 2.03 1.57 1.78 1.71 1.09 1.79 1.20 1.21 1.24 1.27 2.06 1.92 1.55 1.89 1.24 1.37 1.19 1.54 1.97 1.51 | Mixture Mixture Mixture Mixture Mixture 2.21 2.03 1.57 1.30 1.78 1.71 1.09 1.08 1.79 1.20 1.21 1.32 1.24 1.27 2.06 1.54 1.92 1.55 1.89 1.41 1.24 1.37 1.19 1.15 1.54 1.97 1.51 1.66 |

(6) Finally, liquid flow rate in the rectifying section and liquid flow and vapor flow in the stripping section are calcu-

Then the calculations continue for the next distillation column.

Minimum Energy Requirements for Quaternary Systems

Similarly as in ref. 11, various feed compositions and relative volatilities were considered. Relative volatilities were chosen, assuming all combinatorial possibilities of easy splits ($\alpha = 2.5$) and difficult splits ($\alpha = 1.1$) between neighboring components. There are eight combinations: eee, eed, ede, dee, edd, ded, dde, ddd. For example, ede means that AB split is easy (first e), BC split is difficult (d in second position), and CD split is easy (last e).

Five representative feed compositions were chosen: feed rich in component A, B, C, D, and equimolar feed. For a feed rich in a given component, the mole fraction of this component is assumed to be 0.85 and mole fractions of the other components are 0.05.

To reduce the number of results, the calculations were made for three types of configurations: thermally coupled systems (with liquid and vapor streams between the columns), configurations with liquid interconnecting streams only, and configurations with either liquid or vapor connections.

In each of these three categories, the minimum vapor flows were calculated for 22 column configurations, 8 types of splits, and 5 types of feed compositions. Because of space constraints, it would be difficult to report 880 results for each category. Therefore, the results for each category are reported in three types of tables. In the first table there are configurations with the minimum vapor flow within 10% from the optimal configuration. This allows the user to choose the most appropriate configuration from the set of (almost) equivalent, optimal systems. The second table

Table 10. The Ratio of Minimum Vapor Flow of the Best L Configuration to the Minimum Vapor Flow of the **Optimal LV System**

| Split | A-Rich Mixture | B-Rich Mixture | C-Rich Mixture | D-Rich Mixture | M Mixture |
|-------|-------------------|-------------------|-------------------|-------------------|--------------|
| eee | 1.13 | 1.08 | 1.01 | 1.28 | 1.13 |
| eed | 1.40 | 1.18 | 1.00 | 1.02 | 1.09 |
| ede | 1.26 | 1.02 | 1.02 | 1.25 | 1.11 |
| dee | 1.02 | 1.02 | 1.11 | 1.19 | 1.13 |
| edd | 1.32 | 1.06 | 1.03 | 1.13 | 1.29 |
| ded | 1.12 | 1.02 | 1.01 | 1.07 | 1.11 |
| dde | 1.12 | 1.04 | 1.13 | 1.40 | 1.35 |
| ddd | 1.16 | 1.13 | 1.13 | 1.17 | 1.36 |

Table 11. Interconnecting Vapor Streams in SLSV Systems; Feed Number Corresponds to Column Number Where the Feed is Entering

| Configuration | Split Code | Feed Number Where $q = 0$ | Configuration | Split Code | Feed Number Where $q = 0$ |
|---------------|---------------|---------------------------|---------------|---------------|---------------------------|
| a | 101 | | 1 | 422 | 2, 4 |
| b | 102 | 5 | m | 423 | 2, 4 |
| c | 103 | 5 | n | 431 | 2, 4 |
| d | 201 | 4 | 0 | 432 | 2, 4 |
| e | 202 | 4, 5 | p | 433 | 2, 4 |
| f | 203 | 4, 5 | q | 510 | 2 |
| g | 300 | 4 | r | 520 | 2, 4 |
| h | 411 | 2 | S | 530 | 2, 4 |
| i | 412 | 2 | t | 610 | 2 |
| j | 413 | 2 | u | 620 | 2, 4 |
| k | 421 | 2, 4 | V | 630 | 2, 4 |

gives the ratio of minimum vapor flows of the highest and the lowest energy consuming configurations, within a given category. This allows estimating the maximum energy penalty if the distillation system is chosen incorrectly. The third table gives the ratio of minimum vapor flows of the best configuration in the given category to the minimum vapor flow of the optimal thermally coupled system, which gives the estimate of the penalty for not using the thermally coupled configuration.

Thermally coupled configurations (LV systems)

Table 6 lists all the LV configurations with the minimum vapor flow within 10% from the optimal vapor flow. As was shown previously,11 a fully thermally coupled system always has the lowest minimum vapor flow when compared with conventional configurations.

In one entry in Table 6 (for ddd split and equimolar feed), only the fully thermally coupled system (l) uses distinctly less energy than all the other systems. However, for all the other types of splits and feed compositions, there are several alternative optimal thermally coupled systems with energy consumption within 10% (and in many cases, much less than 10%) of the fully thermally coupled system. Therefore, the fully thermally coupled system is usually not the only configuration with minimum energy, and some other thermally coupled configurations can do almost as well. These alternative thermally coupled systems are simpler than the fully thermally coupled configurations, and they may be easier to build and operate.

On the other hand, as shown in Table 7, the ratio of minimum vapor flows of the highest and the lowest energy consuming configurations in the LV group is usually bigger than 1.10. There are only 5 cases where this ratio is less than 1.10. In all other cases, despite the fact that there are usually many thermally coupled systems with similar minimum vapor flow, not all the thermally coupled systems are equivalent (with energy requirements within 10%). If the fully thermally coupled system is replaced with a wrong thermally coupled system, then the energy penalty may be even more than 100%.

Column configurations with two B or C product streams (h,k,n,o) are frequently in the top 10% list, but they never stand out as the systems distinctly better than others.

Configurations with liquid interconnecting streams (L systems)

Table 8 lists all L configurations with the minimum vapor flow within 10% from the optimal L configuration. There are fewer configurations that are close to the optimal configuration than in the LV group.

For the A-rich mixture, a, b, and c configurations are most frequently listed as optimal; for the B-rich mixture, it is configuration d; and for the C-rich mixture, it is configuration l.

Configuration I also appears as the only optimal system in the ddd group for the equimolar feed.

The configurations with two B or C product streams (h,k,n,o) are again frequently in the top 10% list, but they never stand out as the systems distinctly better than others.

Table 9 shows how much minimum vapor flows can differ in the L group. Only in two cases (eed, C and D-rich mixtures) are these differences less than 10%. Therefore, the choice of the proper L system has a significant impact on the energy requirements. By making a wrong choice, one can easily spend 50 or 100% more energy than necessary.

Table 10 lists the ratio of minimum vapor flow of the best L configuration to the minimum vapor flow of the optimal LV system. The highest ratio is 1.40, that is, one can spend 40% more energy by choosing the best L configuration instead of the optimal thermally coupled system. Surprisingly, in 15 out of 40 cases, this ratio is less than 1.10 and in 10 cases it is less than 1.03. Therefore, depending on the feed compositions and the split type, an optimal L configuration can be almost as attractive as a fully thermally coupled system. This is an important finding, since L configurations are much simpler than LV systems and, therefore, they are easier to build and operate.

Configurations with some liquid and some vapor interconnecting streams (SLSV systems)

In the L system all the interconnecting streams are liquids. This is not efficient in a case when the interconnecting stream is a

Table 12. SLSV Configurations with the Minimum Vapor Flow Within 10% from the Optimal SLSV Configuration

| Split | A-Rich Mixture | B-Rich Mixture | C-Rich Mixture | D-Rich Mixture | M Mixture |
|-------|----------------|----------------|----------------|----------------|----------------|
| eee | ALL-(puv) | defknr | iloqrs | uv | eilor |
| eed | egjlkor | defghklnoru | ALL | ALL | ALL |
| ede | defblmnoqr | ALL-(cijpqt) | behiklnoqrs | eqrsuv | ALL-(acjptuv) |
| dee | ALL | defklmnop | lr | egjlr | ALL-(abcpstuv) |
| edd | ebgil | adghkn | beilogrs | cfjmptuv | beilogrs |
| ded | ALL-(puv) | eklmo | ALL-(abcdhtuv) | ALL-(abh) | egjklor |
| dde | abchijqt | def klmru | gnops | lmr | deflmru |
| ddd | abc | d | ils | tuv | 1 |

Listed configurations are denoted by letters as in Figures 2–8. ALL means all configurations.

distillate from the previous column. Such a stream is condensed in a condenser just to be vaporized again in the next column. It may be better to pass such a stream as vapor. To find that out, calculations of minimum vapor flows were made for systems where distillate interconnecting streams were left as vapors. A detailed list of interconnecting vapor streams is given in Table 11.

Indeed, in most cases, SVSL systems require less energy than corresponding L systems. There is no case where an SVSL system would require more energy than the corresponding L configuration.

Table 12 shows SLSV configurations with the minimum vapor flow within 10% from the optimal SLSV configuration. There are multiple SLSV systems within 10% from the minimum power. Again, for the ddd split and equimolar feed, I system is listed as standalone. The configurations with two B or C product streams (h,k,n,o) are again frequently in the top 10% list. In three cases, systems n, k, and h have the lowest power among SLSV configurations. The difference is not big, however—only 2–4%.

The ratio of minimum vapor flow of the worst to the best SLSV configuration is shown in Table 13. This ratio can be more than 2, that is, a more than 100% energy penalty is possible if the wrong choice of SLSV system is made.

Table 14 shows the ratio of minimum vapor flow of the best SLSV configuration to the minimum vapor flow of the optimal LV system. This ratio can be as high as 1.36, but in 17 cases it is lower than 1.10. Therefore, in these cases, building an optimal SLSV system instead of the optimal thermally coupled system would not cause significant energy penalty.

Conclusions

The fully thermally coupled system has lower energy requirements than conventional quaternary configurations. The fully thermally coupled system is especially attractive for the ddd split for the equimolar feed. In other cases, some other (partially) thermally coupled systems may match its energy requirements or their energy consumption is very similar (slightly higher).

Interestingly, for the L-type systems, configuration 4–2-2 (prefractionator system analogous to the fully thermally coupled system) is the most efficient for the separation equimolar feed and ddd split. The best L-system may require 40% more energy than the fully thermally coupled system. However, for some other feed compositions and splits, there exist prefractionator-type arrangements with liquid connections that have energy requirements within 3% of the fully thermally coupled system.

Table 13. The Ratio of Minimum Vapor Flow of the Worst to the Best SLSV Configuration

| Split | A-Rich Mixture | B-Rich Mixture | C-Rich Mixture | D-Rich Mixture | M Mixture |
|-------|-------------------|-------------------|-------------------|-------------------|--------------|
| eee | 1.16 | 2.03 | 1.53 | 1.42 | 1.65 |
| eed | 1.32 | 1.67 | 1.08 | 1.08 | 1.09 |
| ede | 1.31 | 1.19 | 1.22 | 1.40 | 1.18 |
| dee | 1.07 | 1.28 | 2.02 | 1.57 | 1.18 |
| edd | 1.46 | 1.54 | 1.89 | 1.43 | 1.45 |
| ded | 1.14 | 1.38 | 1.18 | 1.14 | 1.81 |
| dde | 1.39 | 1.96 | 1.52 | 1.74 | 1.52 |
| ddd | 1.59 | 2.18 | 2.09 | 1.65 | 1.88 |

Table 14. The Ratio of Minimum Vapor Flow of the Best SLSV Configuration to the Minimum Vapor Flow of the **Optimal LV System**

| Split | A-Rich Mixture | B-Rich Mixture | C-Rich Mixture | D-Rich Mixture | M Mixture |
|-------|-------------------|-------------------|-------------------|-------------------|--------------|
| eee | 1.11 | 1.05 | 1.01 | 1.13 | 1.13 |
| eed | 1.18 | 1.18 | 1.00 | 1.01 | 1.08 |
| ede | 1.13 | 1.02 | 1.01 | 1.18 | 1.06 |
| dee | 1.02 | 1.00 | 1.10 | 1.15 | 1.05 |
| edd | 1.25 | 1.06 | 1.03 | 1.12 | 1.29 |
| ded | 1.06 | 1.01 | 1.01 | 1.07 | 1.10 |
| dde | 1.11 | 1.04 | 1.11 | 1.33 | 1.28 |
| ddd | 1.16 | 1.13 | 1.12 | 1.16 | 1.36 |

Configurations with liquid connections originating from the reboilers and vapor connections from the condensers are even more efficient than L systems. In many cases, their energy is very close to the fully thermally coupled system.

Total cost (including capital and operating cost) is usually proportional to the minimum vapor flow of a given configuration of distillation columns. In some cases, where column stacking is involved, some column sections may operate much above the minimum reflux. In these cases, detailed evaluation of capital costs may be necessary.

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Notation

A, B, C, D, E = component A, B, C, D, Eq = feed quality α_i = relative volatility of component i I, II, III, IV, V, $V\dot{I} = \text{column number}$

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