Synthesis of Multicomponent Distillation Column Configurations

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A systematic procedure presented here draws distillation column configurations to separate an ideal to near ideal $n-$component mixture into n product streams with each enriched in one of the components. The method synthesizes all feasible basic configurations using $n-1$ distillation columns with each column having only a condenser at the top and a reboiler at the bottom. It also generates all feasible thermally coupled schemes with classical two-way liquid and vapor communication between the distillation columns. The method is simple and easy to use. The advantage of such a method is that it could be incorporated in a search algorithm to systematically find an optimum distillation scheme for a given application.

Introduction

Distillation column configurations to separate a feed mixture containing three or more components into pure product streams have been studied for quite some time. Textbooks by King (1980) and Henley and Seader (1981) discuss algorithms to draw all possible configurations using sharp splits between components of adjacent volatilities. Such schemes are generally referred to as having direct or indirect splits. Thompson and King (1972) presented an equation to calculate the number of such possible sequences for the separation of an $n-$component mixture into single-component product streams. Some other known configurations include schemes similar to the prefractionator configuration for a ternary feed mixture. Thermally coupled configurations with reduced numbers of reboilers and condensers have also been proposed. Some examples include: Seidel (1935), Cahn and DiMiceli (1962), Pelyuk et al. (1965), Sargent and Gaminibandara (1976), Agrawal (1996a), and Agrawal and Fidkowski (1999a).

Multicomponent distillation superstructures with the claim of containing almost all possible configurations have been suggested in the past (Sargent and Gaminibandara, 1976; Hu et al., 1991; Agrawal, 1996a). A "state task network" to draw configurations by assigning tasks in steps, starting from a given feed, was recently proposed by Sargent (1998). Other researchers (Yeomans and Grossmann, 1999; Caballero and Grossmann, 2001; Doherty and Malone, 2001) have made additions and modifications to the formalism of Agrawal (1996a) and Sargent (1998). Although past work on multicomponent distillation configurations has generated a large body of extremely valuable information, a systematic procedure has not yet been published to generate all possible distillation configurations for a given $n-$component mixture. A method that could systematically draw thermally coupled, as well as nonthermally coupled, schemes would be quite useful in searching for the optimum configuration for a specific multicomponent separation. The purpose of this article is to report one such procedure.

For the purpose of this article, all possible distillation configurations will be divided into two categories—*basic* and *thermally coupled*. For an $n-$component mixture, each configuration in the basic category uses $n-1$ distillation columns, with a reboiler at the bottom and a condenser at the top of each column. A distillation column is allowed, however, to contain more than two sections. A column section is defined to be a portion of a distillation column, which is not interrupted by entering or exiting streams, or heat flows (Hohmann et al., 1982). The basic configurations do not contain two-way material flow communications as found in the thermally coupled distillation configurations. A mixture containing the same group of components is transferred only once from one distillation column to another. A product stream enriched in one of the constituents of the feedstream is produced only once. Thus, configurations where product streams enriched in the same component are recovered from two or more distillation columns are not included in the basic configurations (Agrawal, 2000a). Such configurations are later

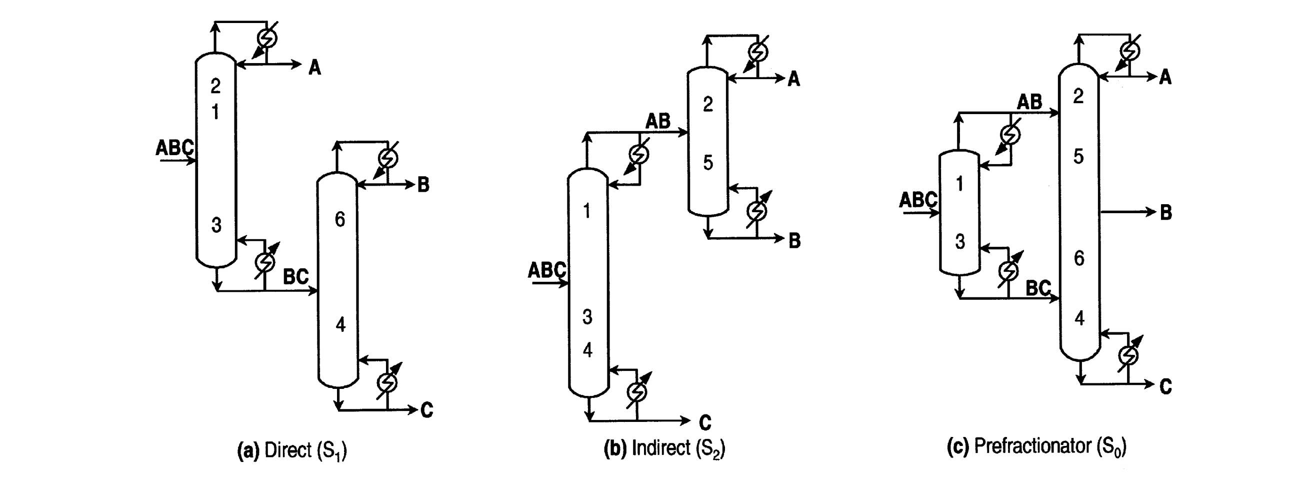

Figure 1. Basic configurations for a ternary distillation.

classified as derived-thermally coupled configurations. Figure 1 shows all the basic distillation configurations for a ternary feed mixture *ABC*. In these figures, and throughout this article, components in a mixture are ranked according to their relative volatility, that is, for feed mixture *ABC*, *A* is the most volatile component and volatility decreases in successive order, with *C* being the least volatile.

The second broad class of distillation configurations is thermally coupled. A thermal coupling requires a two-way communication between the two distillation columns. In a

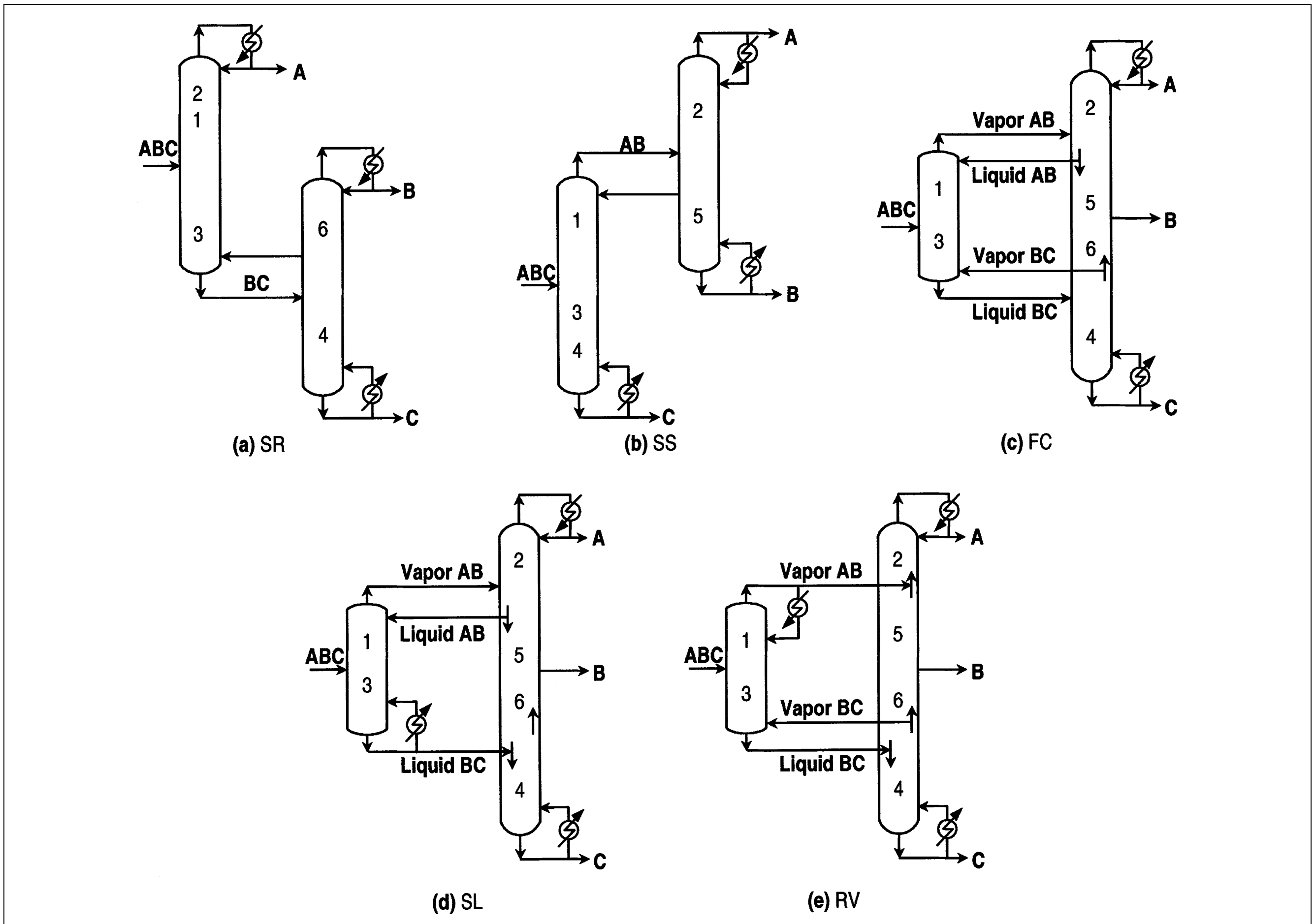

Figure 2. Distinct thermally coupled configurations for a ternary distillation.

two-way communication, when a vapor stream is sent from one column to another column, a return liquid stream is then implemented between the same locations of the two columns. Figure 2 shows all of the *distinct* thermally coupled configurations for a ternary feed mixture. For any n−component mixture, it has been shown that all the side stripper and side rectifier configurations can be derived by replacing mixture reboilers or condensers in the basic configurations containing only sharp splits with two-way communications (Agrawal, 1996a). For example, the side rectifier in Figure 2a is obtained by eliminating reboiler *BC* in Figure 1a and replacing it with two-way communication between the columns. Other thermally coupled configurations, such as the SL, RV, and fully coupled schemes in Figure 2, are derived by eliminating one or both of reboiler *BC* and condenser *AB* from the prefractionator scheme in Figure 1c. It is clear that all the distinct ternary thermally coupled configurations can be derived from the basic configurations of Figure 1.

Once all the distinct thermally coupled configurations are known, then for each of the distinct configuration, all the thermodynamically equivalent configurations can be easily drawn (Agrawal, 1999, 2000b). This is achieved by moving an appropriate distillation section from one column to the other column. For example, the familiar side rectifier configuration can be easily obtained from Figure 2a by moving section 4 and the associated reboiler *C* to underneath section 3. The resulting familiar side rectifier configuration is thermodynamically equivalent to the one in Figure 2a. Both will have the same heat duty. Therefore, during the search for an optimum solution, it may be of interest to reduce the search space by excluding the thermodynamically equivalent configurations. This will often lead to considerable reduction in the computational effort. While the heat duty between the thermodynamically equivalent configurations is expected to be similar, the differences between different column heights and the variation in column diameters can lead to some cost differences. When such cost differences are important, it will be beneficial to examine the thermodynamically equivalent configurations of the optimum configuration obtained from the reduced search space. However, the major interest in the thermodynamically equivalent configurations arises from the perspective of operability. When an optimum distinct thermally coupled configuration drawn from a basic configuration has the classical vapor transfer problem between the distilla-

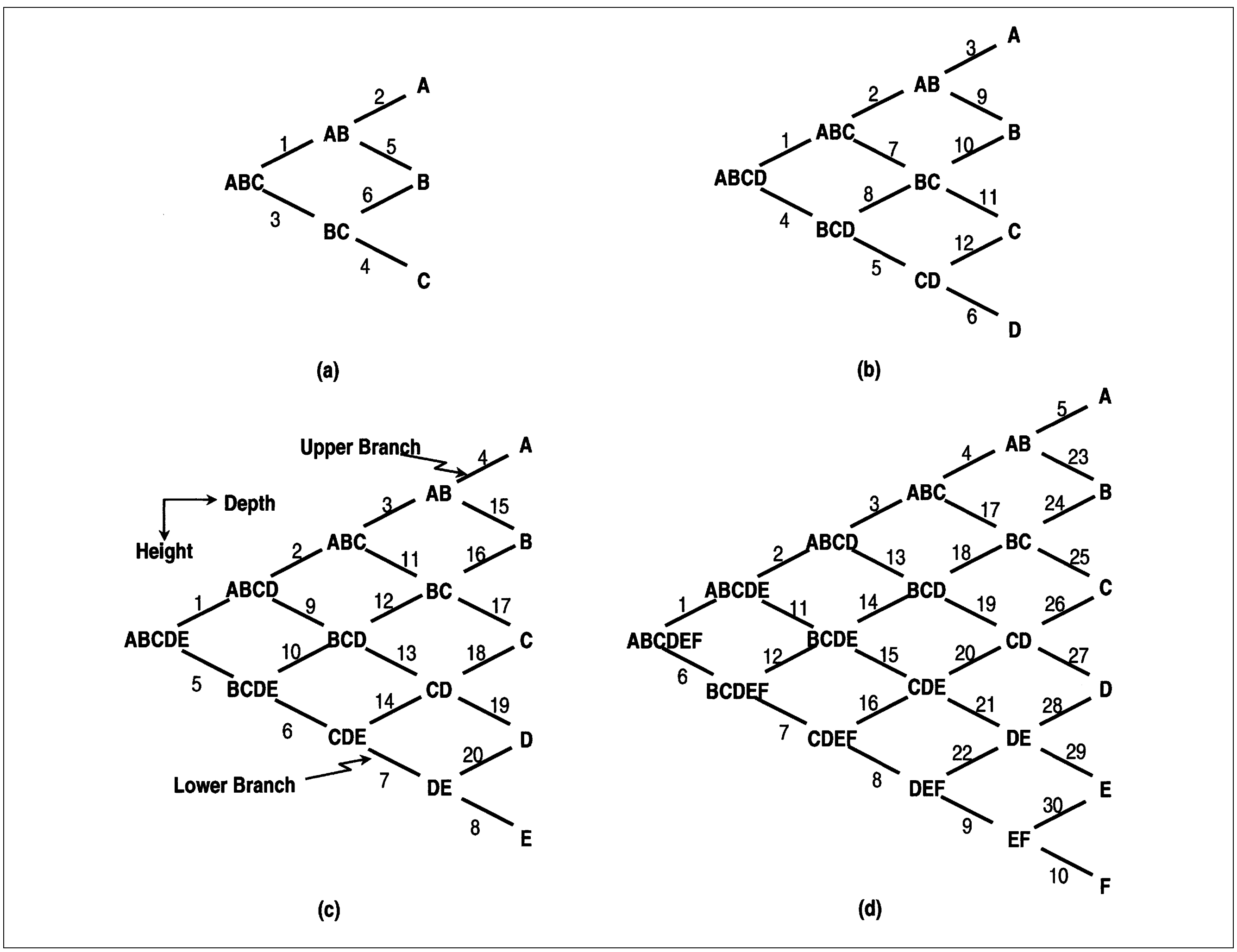

Figure 3. Network representation for the separation of (a) three, (b) four, (c) five and (d) six-component mixtures.

tion columns, then a thermodynamically equivalent configuration can eliminate such a problem (Agrawal, 1999). The fully coupled configuration in Figure 2c is such an example. On the basis of the previous observations, it can be said with confidence that, for every distinct thermally coupled configuration, a thermodynamically equivalent easy to operate configuration can be easily drawn (Agrawal, 1999, 2000b). Thus, an optimization problem may involve the search among only the basic and the distinct thermally coupled configurations, and, if subsequently needed, it can be followed with an exercise to draw more operable thermodynamically equivalent configurations.

In this article, we first describe a systematic method to generate all possible basic distillation configurations for any n–component feed mixture. A procedure is then described on how to derive distinct thermally coupled configurations from the known basic schemes. For an optimization task at hand, the method provides a much better search space of distillation configurations. Finally, a brief discussion is presented on column arrangements that can be derived from these thermally coupled configurations.

Basic Multicomponent Distillation Configurations

This section presents a method to draw all of the feasible basic distillation configurations for an n–component mixture. Only mixtures with near-ideal vapor-liquid equilibrium relationships are considered. Each of these schemes uses $n-1$ distillation columns, and each column has a condenser on the top and a reboiler at the bottom. No intermediate reboilers or condensers are used. Therefore, the total number of reboilers and condensers is each equal to $n-1$. Because each component-rich stream is recovered from only one location in the flowsheet, the total number of product streams recovered from a basic distillation configuration is equal to n, the number of components in the feed mixture. Furthermore, from any basic distillation configuration, each of the n components can be recovered at any desired high purity with finite refluxes in the distillation columns. As a result, configurations, such as a single distillation column with a ternary feed mixture ABC where B is recovered as a sidestream from an intermediate location of the distillation column, are not included within the "basic configuration" category. A submixture containing the same group of components is transferred only once from one distillation column to another. There is no two-way communication between the columns, that is, no thermally coupled columns are included. The total number of column sections in basic distillation configurations vary from the minimum of $2(n-1)$ to the maximum of $n(n-1)$. The three known basic distillation configurations for a ternary feed mixture are shown in Figure 1.

In order to draw all possible basic configurations, it is convenient to start from a network representation of an n–component distillation (Sargent and Gaminibandara, 1976; Hu et al., 1991; Agrawal, 1996a, 2000b; Sargent, 1998). In this article we follow the network description used by Agrawal (2000b). Figure 3 shows network representations for three, four, five, and six-component mixtures. In any given network, the feed mixture is represented by the "root" node. The root, the intermediate nodes, and all of the final product nodes represent distinct mixtures. A mixture at an intermediate node is a feasible "submixture" from the feed; its presence at a node indicates that it is transferred from one distillation column to another distillation column, in order to be further separated into two submixtures. A line connecting a node with a successive node represents a section of a distillation column. "Complete networks" such as those in Figure 3 have $n(n+1)/2$ different submixtures including the feed, and a total of $n(n-1)$ distillation sections. All of the feasible submixtures for any feed can be easily identified and rank listed (Rathore et al., 1974; Henley and Seader, 1981). The position in the network of various submixtures of the initial mixture is automatically specified through the use of the rank list.

The location of a submixture within the n–component network can be specified by defining its "depth" and "height" (Agrawal, 2000b). The root (or feed) node is at a depth of one, while the terminal (or product) nodes are said to be located at the depth n. Each of the m submixtures located at depth m have $(n-m+1)$ components. For example, in Figure 3c for a five-component network, there are four submixtures located at the depth of 4 (that is, $m=4$) and each of these is a binary mixture. The upper branch in a network consists of all the submixtures that contain the most volatile component A, and the lower branch consists of all the submixtures containing the least volatile component of the feed mixture. Those submixtures that are not members of either the upper branch or the lower branch, and contain only components with intermediate volatilities are defined as *internal submixtures*. By this definition, pure products of intermediate volatility are also defined as internal submixtures. The term *intermediate product* is used to describe a product stream of intermediate volatility. At a given depth, the height of a submixture is measured from the submixture on the upper branch. At depth m, the submixture on the upper branch is assigned a height of one while the submixture on the lower branch is assigned a height of m. Thus, the binary mixture CD in the network of Figure 3c is located at the depth of four and height of three. This coordinate system uniquely and conveniently locates the position of all the submixtures within a network.

For an n–component mixture, once the network representation for distillation is drawn and characterized, one can begin the task of drawing all possible basic configurations.

Method to draw basic distillation configurations

In the method to be described below, first, each product of intermediate volatility is assigned to be associated with a reboiler, a condenser, or neither. All possible options of these assignments are then generated. For each possible option, the n–component network problem is reduced to an $(n-1)$–component network problem through a systematic stepwise procedure. From the prior knowledge of $(n-1)$–component configurations, the configurations for the n–component mixture can then be derived. The method is based on the premise that all the basic configurations for a three-component mixture are known and are given in Figure 1. Thus, the four-component configurations are derived first, followed by the five-component mixture and so on. This allows the creation of all feasible basic configurations for any given multicomponent mixture. The stepwise procedure is based on nine observations. Therefore, these observations are developed below first, followed by a description of the stepwise procedure that incorporates these observations.

Observation No. 1. *The lightest component (A) is always recovered from the top of a distillation column and has an associated condenser. Conversely, the heaviest component is always recovered from the bottom of a distillation column with an associated reboiler.*

Observation No. 2. *A component of intermediate volatility may be recovered with an associated condenser or a reboiler or neither of the two.* For a ternary mixture *ABC*, direct split is an example where *B* is recovered from a condenser, indirect split is an example where *B* is recovered from a reboiler, and in the prefractionator scheme, *B* is recovered from an intermediate location of a distillation column without any associated condenser or reboiler (Figure 1).

Observation No. 3. *Whenever a submixture is associated with a condenser or a reboiler, this submixture is always withdrawn from the distillation column.* If this submixture is not recovered as a product stream, then it must be transferred to another distillation column. Since no intermediate reboilers or condensers are used in a basic configuration, such submixtures are withdrawn either from the top or the bottom of a distillation column. In Figure 1a, binary mixture *BC* is an example of such a submixture.

Observation No. 4. *If a submixture is transferred from one distillation column to another distillation column, then both the sections emanating from it are needed and they exist in the distillation column receiving the submixture.* (Note: final product streams are not transferred between distillation columns.) In a network, there are four sections associated with any internal submixture that is composed of more than one component. Two of these sections lead to this submixture from an earlier depth (leading sections) and the other two emanate to the next depth (emanating sections). For example in Figure 3c, sections 13 and 14 are leading sections for binary mixture *CD* (from a depth of three), while sections 18 and 19 are emanating sections from *CD* that emanate to pure products at the depth of five. (Note that any section may be described as "emanating" from its upstream node and "leading" to its downstream node. Therefore, the discussion of "emanating" and "leading" is in context of the submixture under discussion.) According to this observation, in Figure 1a when binary submixture *BC* is transferred to the second distillation column, this column then has a section above and a section below the feed point of submixture *BC* (both the emanating sections 6 and 4).

Observation No. 5. (a) *When a submixture on the upper branch is transferred from one distillation column to another, then it has a condenser associated with it at the withdrawal location.* In Figure 1b, transfer of binary submixture *AB* from the top of the first column is such an example. If the first column distilled *A* from the top and the binary submixture *AB* were to be withdrawn from an intermediate location of this first column, then, in conjunction with observation No. 4, two product streams rich in component *A* (one from top of each column) would be produced. We have precluded such configurations from the basic configurations. (A corollary of this observation is that recovery of a submixture on the upper branch is always associated with the use of a condenser.) (b) *Conversely, when a submixture on the lower branch is transferred from one distillation column to another then it has a reboiler associated with it at the withdrawal location.* (A corollary of this observation is that recovery of a submixture on the lower branch is always associated with the use of a reboiler.) In Figures 1a and 1c, transfer of binary submixture *BC* is such an example. (c) *An internal submixture, which is neither on the upper nor the lower branch, can be transferred between the columns with or without an associated reboiler or condenser.* When it is withdrawn from an intermediate location of a distillation column, then there is no associated reboiler or a condenser.

Observation No. 6. (a) *When a condenser is associated with an internal submixture at a depth m in a network, then transfers of all submixtures are eliminated at depths earlier than m that contain the internal submixture as the heavy subgroup within the submixture.* For example, in the Figure 3a network, when a condenser is used with internal submixture *B* at depth three, then binary submixture *AB*, at depth two that contains *B* as the heavy subgroup within *AB*, is not transferred between the distillation columns. When a submixture is not transferred between the distillation columns, then its presence within the network is eliminated (product streams are exceptions). For the example problem, the resulting configuration is the direct split configuration in Figure 1a. In this configuration, if submixture *AB* were to be transferred, then component *B* would have to be subsequently recovered from this stream and this could not be achieved through the use of a condenser. It has already been decided, however, that a condenser is to be used with *B*, and, in a basic configuration, *B* can be recovered from only one location in the configuration. (b) *Conversely, when a reboiler is associated with an internal submixture at depth m, transfer of all submixtures at depths earlier than m that contain the internal submixture as the light subgroup within the submixture are eliminated.* For example, in the Figure 3a network, when a reboiler is used with internal submixture *B* at depth three, then binary submixture *BC* at depth two that contains *B* as the light subgroup is not transferred between the distillation columns. The indirect split configuration in Figure 1b is such an example. (c) *Finally, for the recovery of an internal submixture at depth m from a distillation column without an associated reboiler or a condenser, there must be distillation sections both above and below the withdrawal point.* The distillation section above this point must be fed with a submixture that contains the internal submixture as the heavy subgroup. Similarly, the distillation section below this point must be fed with a submixture that contains the internal submixture as the light subgroup. The prefractionator configuration in Figure 1c presents an example of this concept. The internal submixture *AB* containing *B* as the heavy group is fed to the section above the withdrawals location of *B*. The internal submixture *BC* containing *B* as the light subgroup is fed to the section below the withdrawal location of *B*. It is worth noting that the submixture to be fed to the distillation sections above or below the withdrawal location of the internal submixture may originate at any depth that is earlier than the depth of m.

Observation No. 7. This observation is a corollary of observation 6c. Consider an internal submixture at a depth m that is recovered from a distillation column using a condenser. Then, there must be a section below the withdrawal location, and this section is fed by a submixture that contains the internal submixture as the light subgroup, and this sub-

Table 1. Basic Distillation Configuration Options for a Four–Component Mixture

Options	Shortcut	Applicable Ternary Options	No. of Config. N_{BC}
S_{00}	$ABCD \rightarrow \phi\phi\phi$	$S_\phi + S_3$	4
S_{01}	$AB\overline{C}D \rightarrow AB\phi$	S_0	1
S_{02}	$AB\underline{C}D \rightarrow \phi\phi D$	S_ϕ	3
S_{10}	$A\overline{B}CD \rightarrow A\phi\phi$	S_ϕ	3
S_{11}	$A\overline{B}\overline{C}D \rightarrow A\overline{B}\phi$	S_1	1
S_{12}	$A\overline{B}\underline{C}D \rightarrow A\phi D$	S_ϕ	3
S_{20}	$A\underline{B}CD \rightarrow \phi CD$	S_0	1
S_{21}	$A\underline{B}\overline{C}D \rightarrow A\underline{B}\phi$	S_2	1
S_{22}	$A\underline{B}\underline{C}D \rightarrow \phi\underline{C}D$	S_2	1
			$S_{\phi\phi} = 18$

mixture originates from a depth earlier than m. Similarly, consider an internal submixture at depth m that is recovered from a distillation column using a reboiler. There must now be a section above the withdrawal location and this section must be fed by a submixture that contains the internal submixture as the heavy subgroup, and this submixture originates from a depth earlier than m.

Based on above observations, a stepwise procedure can be created to draw basic distillation configurations for the separation of a given n−component mixture.

Step 1. Following observations 1 and 2, the first step is to generate all possible options with assignments of reboilers and condensers to the products of intermediate volatility. For a ternary feed mixture ABC, there are three feasible options: (1) No reboiler or condenser at B, (2) A condenser at B, and (3) A reboiler at B. When $n > 3$, there are $n-2$ products of intermediate volatility and three possibilities exist for each of these products. This leads to a total of $3^{(n-2)}$ possible options. Table 1 lists nine possible options for a four-component mixture. In this work a notation is adopted to uniquely identify each option. Symbol "S" with $n-2$ subscripts, one for each product of intermediate volatility, is used. The first subscript (left-most one) is associated with the second most volatile product and the volatility decreases in successive order with the last subscript referring to the second least volatile product. Each subscript is allowed to take one of three (0, 1, and 2) values. The subscript 0 indicates that no reboiler or condenser is present, 1 indicates presence of a condenser, and 2 indicates the presence of a reboiler. Thus, in Table 1, S_{ij} uniquely identifies each of the options for a four-component mixture. Subscript i refers to component B and j to component C. S_{00}, for example, means no reboiler or condenser at either B or C. S_{12} implies a condenser at B and a reboiler at C, and so on.

Step 2. Once each n−component option is uniquely identified, each one is then reduced to the corresponding $(n-1)$−component network options and all possible distillation configurations are created.

For a three-component mixture, there are only three options: S_0, S_1, and S_2. For option S_0, no reboiler nor condenser is associated with B and observation 6c suggests that binary submixtures AB and BC must be transferred to the distillation column producing B. From observation 5, a condenser is associated with the recovery of AB and a reboiler with the recovery of BC. Therefore, when one looks at the depth of two, this option reduces to an equivalent binary network option, that is, a single distillation column with a feed and a condenser at the top for AB and a reboiler at the bottom for BC. This, in conjunction with observation 4, leads to the prefractionator scheme of Figure 1c. Similarly, for option S_1, use of a condenser at B eliminates submixture AB (from observation 6a) and a reboiler must be used at BC (from observations 7 and 5b). The resulting network is shown in Figure 4a. Note that as submixture AB is eliminated from the network 3a, component A is moved from the depth of three to the depth of two in the network 4a. This is done to first create feasible distillation configurations by considering the network up to the depth that is one less than the depth of the original problem. Therefore, just looking at the depth of two in Figure 4a, option S_1 is again reduced to an equivalent binary network option. This means a distillation column with feed ABC and a condenser for component A and a reboiler for BC. This is, of course, the direct split shown in Figure 1a. Similarly, the network for option S_2 is shown in Figure 4b and it corresponds to indirect split (Figure 1b). *In Figure 4 and all other modified network figures, an overhead line represents a condenser and an underline represents a reboiler.* Thus, the total number of basic configurations S_ϕ for a ternary mixture is equal to three. (Note in this article a subscript ϕ to S denotes that S with all feasible values of 0, 1 and 2 as subscript are considered. Thus S_ϕ represents all possible options for a ternary mixture and $S_\phi = S_0 + S_1 + S_2$. Just as the numerical value of S_i represents the total number of basic distillation configurations for option S_i, similarly, the numerical value of S_ϕ represents the total number of basic distillation configurations for all the options contained in S_ϕ.)

All the nine options for the assignment of reboilers and condensers to the products of intermediate volatility ($=3^{4-2}$) for a four-component mixture are listed in Table 1. There are 27 ($=3^{5-2}$) such options for a five-component mixture. When the number of components is greater than three it is easier to subdivide Step 2 into the following six cases:

Case a. This case occurs when in the option under consideration only one intermediate product stream uses a condenser and the other intermediate products use neither a reboiler nor a condenser. For the purpose of illustration, consider the five-component network in Figure 3c with an associated condenser at C and no associated reboiler or condenser at B or D (option S_{010}). In this option, ABC and BC are the two submixtures at depths earlier than five that contain C as the heavy subgroup. These two submixtures are circled in Figure 5a. According to observation 6a, these circled submixtures are then eliminated resulting in the network shown in Figure 5b. Next, the resulting empty slots are filled by moving appropriate submixtures from greater depths. An empty slot is filled by moving all the submixtures at greater depths, but at the same height by one unit to the left in the network. Therefore, in Figure 5b, each of the submixtures AB and A on the upper branch, that are at the same height as ABC but at greater depths than ABC in the network, are moved one unit to the left. Thus, AB fills in the empty slot of ABC and A in turn fills the vacated slot of AB. Similarly, B fills in the empty slot of BC. The resulting modified network is shown in Figure 5c. The modified networks for the other two options S_{100} and S_{001}, when only one intermediate product has an associated condenser and the other two intermediate

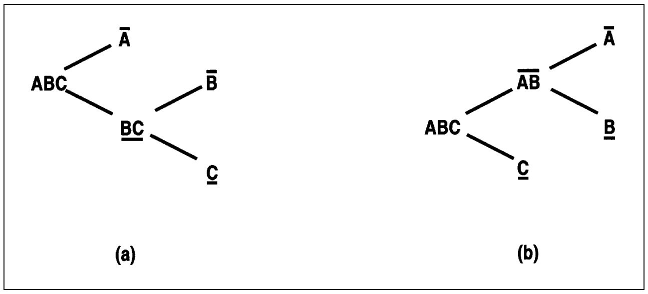

Figure 4. Network representation for a ternary mixture (a) condenser at *B*, and (b) reboiler at *B*.

products neither have a reboiler nor condenser, are shown in Figures 5d and 5e. It is worthwhile to note that, in all the three resulting modified networks, the product streams that are lighter than the intermediate product stream with the condenser are now located at the depth of four and all other product streams remain at the original depth of five.

The modification of an n–component network translates the given option to the corresponding $(n-1)$–component network options. All the decisions to assign reboilers and condensers are now confined to the depths of $n-1$ or earlier. Let us illustrate this point through an option for a four component mixture S_{10}, that is, the use of a condenser at B. The resulting modified network is shown in Figure 6a. Since no reboiler or condenser is used at C, from observation 6c, submixture CD must be transferred and fed to the distillation column producing C. From observation 5b, a reboiler is associated with the transfer of CD. Recovery of C also requires that at least one of the submixtures ABC or BC must be fed to the column producing C (observation 6c). However, BC cannot be eliminated from the modified network as submixture ABC contains B and cannot produce only A and C (observation 8, which will be described below, tells when an internal submixture can be eliminated from the network). As a result, the modified network of Figure 6a at depth three incorporates the earlier ternary separation options, with a condenser at A, a reboiler at CD, and the recovery of BC for transfer to another distillation column. At BC, one again has a choice to use a reboiler, a condenser, or neither. Therefore, up to the depth of three of the modified network, the structure of distillation configurations will be identical to those for the ternary mixture options S_2, S_1, and S_0. This results in the number of configurations at depth three of the modified network for option S_{10} to be equal to $3(=S_{\phi})$. The final four-component configurations are created by adding the production of B, C, and D to each of the equivalent ternary configurations in Figure 1. The resulting three configurations

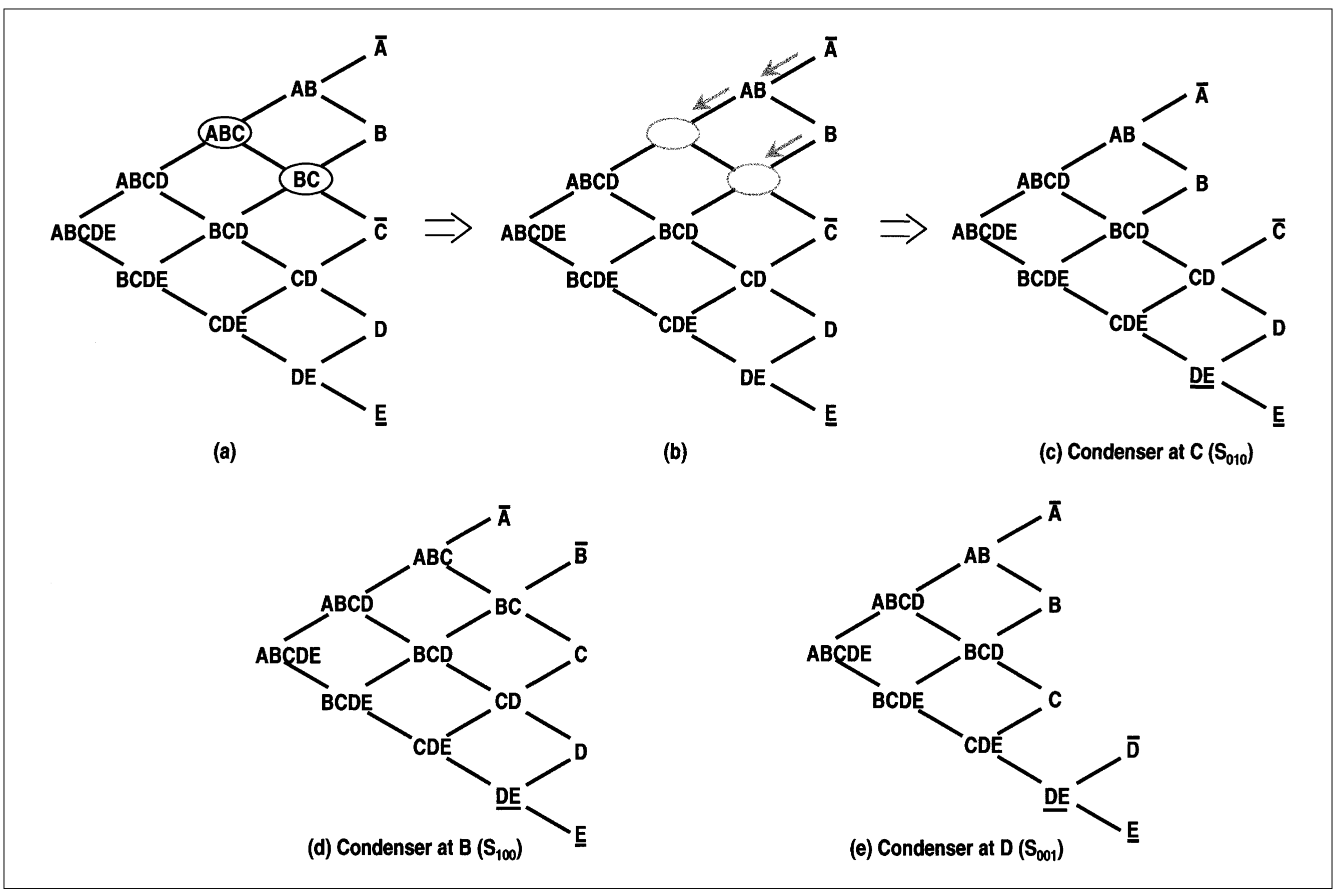

Figure 5. (a)–(c) Modification of a five-component network to eliminate submixtures *ABC* and *BC* in option S_{010}; modified networks for options (d) S_{100} and (e) S_{001}.

are shown in Figures 7i, 7j and 7k (in order not to clutter the figures, condensers are depicted as filled circles and reboilers as open circles).

Now consider option S_{01} in Table 1. The use of a condenser at C in the network of Figure 3b eliminates submixtures BC and ABC from the network (observation 6a). The resulting modified network is shown in Figure 6b. We already now know that binary submixture CD must be recovered using a reboiler and transferred to a distillation column producing C and D (observations 7 and 5b). In the S_{01} option, no reboiler or condenser is associated with B. Therefore, in the modified network of Figure 6b at the depth of three, the only equivalent ternary option applicable is S_0. The resulting configuration for this option is readily obtained by adding the production of C and D to the equivalent ternary option S_0 (prefractionator in Figure 1c) and is shown in Figure 7e.

Case b. Consider the options where only one intermediate product stream uses a reboiler and the other intermediate products use neither a reboiler nor a condenser. Once again for an illustration purpose, consider the five-component network in Figure 3c with an associated reboiler at C and no associated condenser or reboiler at B or D (option S_{020}). In this option, CDE and CD are two submixtures at depths earlier than five that contain C as the light subgroup. These two submixtures are circled in Figure 8a. According to observation 6b, these circled submixtures are then eliminated resulting in the network shown in Figure 8b. An empty slot is filled by moving an adjacent submixture from a depth and height each one unit greater than the depth and height of the empty slot. The adjacent vacated slot is then similarly filled, and the process is continued until all the submixtures up to the depth of five have been appropriately moved. Therefore, submixture DE fills in the empty slot of CDE and E in turn fills the vacated slot of DE. Similarly, D fills in the empty slot of CD. The resulting modified network is shown in Figure 8c. The modified networks for the other two options S_{200} and S_{002} are shown in Figures 8d and 8e. It is observed that, in all the three resulting modified networks, the product streams that are heavier than the intermediate product stream with the reboiler are now located at the depth of four and all other product streams remain at the original depth of five.

In the modified networks, all the decisions to assign reboiler and condensers are confined to the depths of $n-1$ or earlier. This helps to draw n-component configurations from

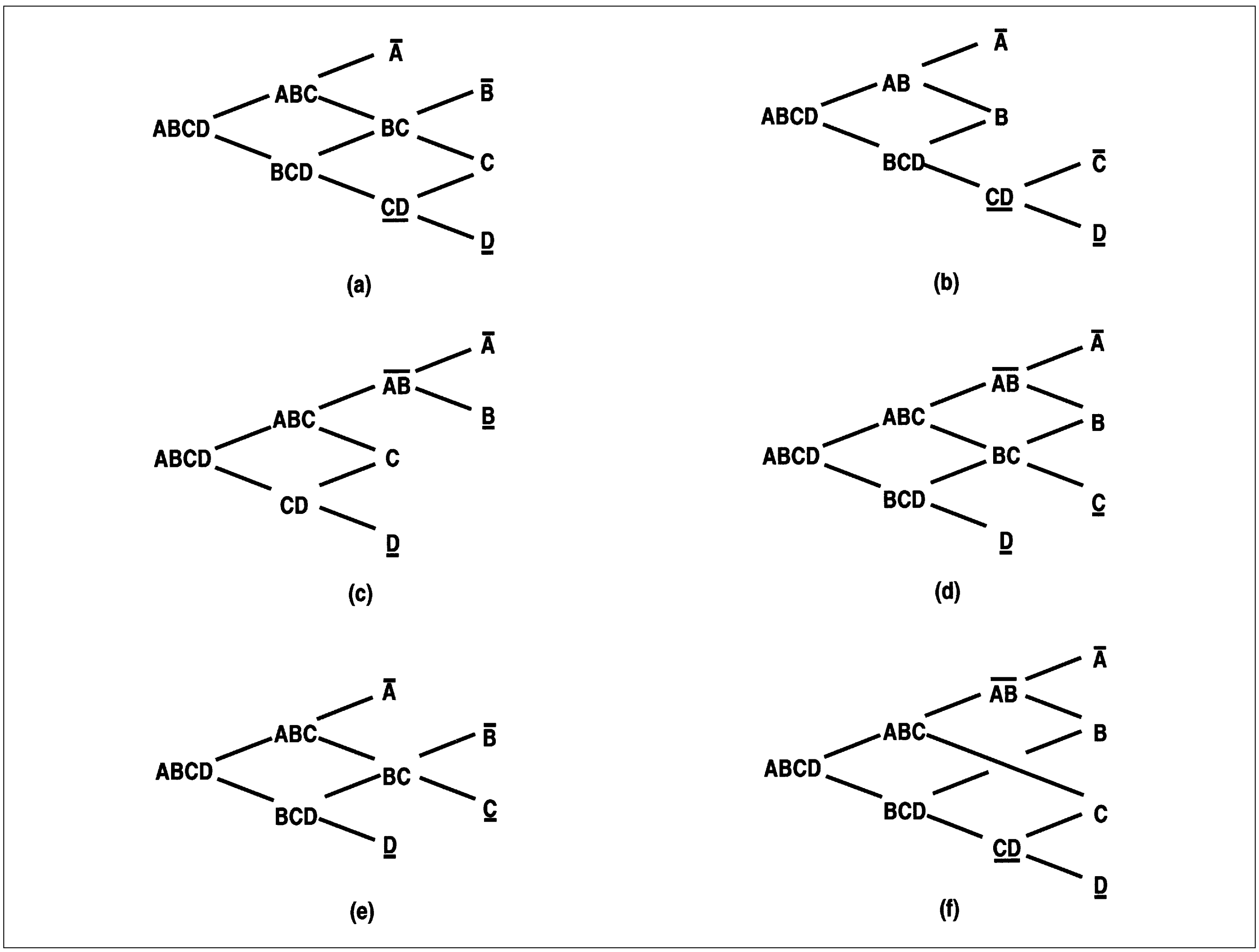

Figure 6. Modified network representations for a four-component mixture.

(a) Condenser at B (S_{10}); (b) condenser at C (S_{01}); (c) reboiler at B (S_{20}); (d) reboiler at C (S_{02}); (e) a condenser at B and a reboiler at C (S_{12}); (f) a solution with no reboiler or condenser at B or C.

the ones available for the $(n-1)$–component. For illustration, consider option S_{20} with a reboiler at B from the four-component mixture options summarized in Table 1. For this option, the resulting modified network is shown in Figure 6c. At the depth of three, a condenser is used for AB, a reboiler for D and no reboiler or condenser for C. Therefore, for up to the depth of three, an equivalent ternary configuration for option S_0 is chosen and the production of A and B is added to it. The one resulting configuration is shown in Figure 7p. In option S_{02}, a reboiler is used at C. This eliminates the submixture CD and results in the modified network of Figure 6d. Once again, a condenser is used at AB (observations 6c and 5), a reboiler at D, and one has all three possible choices for the binary mixture BC. This leads to the number of equivalent ternary network options applicable equal to S_ϕ at the depth of three. The resulting three configurations for a four-component mixture are shown in Figures 7f, 7g, and 7h.

The resulting four-component network options for each of the five-component modified networks shown in Figures 5c–5e and 8c–8e are discussed later in this article.

Case c. Now consider the options where more than one intermediate product stream uses a condenser, but no intermediate product stream uses a reboiler. For a four-component mixture, option S_{11} is such a case. In such cases, pick the heaviest intermediate product with an associated condenser and modify the network according to the steps described for Case a. This will modify the network by moving all the intermediate product streams lighter than the heaviest intermediate product stream with the condenser to the depth of $n-1$. Now, the equivalent options of the $(n-1)$–component network applicable to this n–component option can be easily generated by applying the remaining condensers to the intermediate product streams located at the depth of $n-1$ in the modified network. For option S_{11}, it means to first apply associated condenser to the intermediate product C and modify the network in Figure 3b to obtain modified network S_{01} of Figure 6b. The use of a condenser at B leads to the equivalent ternary network option S_1 (direct split in Figure 1a) at the depth of three. The resulting configuration is obtained by adding production of C and D to the equivalent ternary configuration and is shown in Figure 7l.

Case d. Now consider the options where more than one intermediate product stream uses a reboiler, but no intermediate product stream uses a condenser. For a four-component mixture, S_{22} is such an option. In such options, pick the lightest intermediate product with the reboiler and modify the network according to the steps described for case b. This will modify the network by moving all of the intermediate product streams that are heavier than the lightest intermediate product stream with the reboiler to the depth of $n-1$. The applicable equivalent options for the depth of $n-1$ can now be easily generated by applying the remaining reboilers to the intermediate product streams. For option S_{22}, it means using modified network S_{20} (Figure 6c). At the depth of three, binary submixture AB uses a condenser, D uses a reboiler and C is specified to use a reboiler. This leads to the distillation configuration of ternary option S_2 being applicable; the resulting configuration is shown in Figure 7r.

Case e. Now consider those options where both reboilers and condensers are used by the intermediate product streams. S_{12} and S_{21} from Table 1 are examples of this type of option.

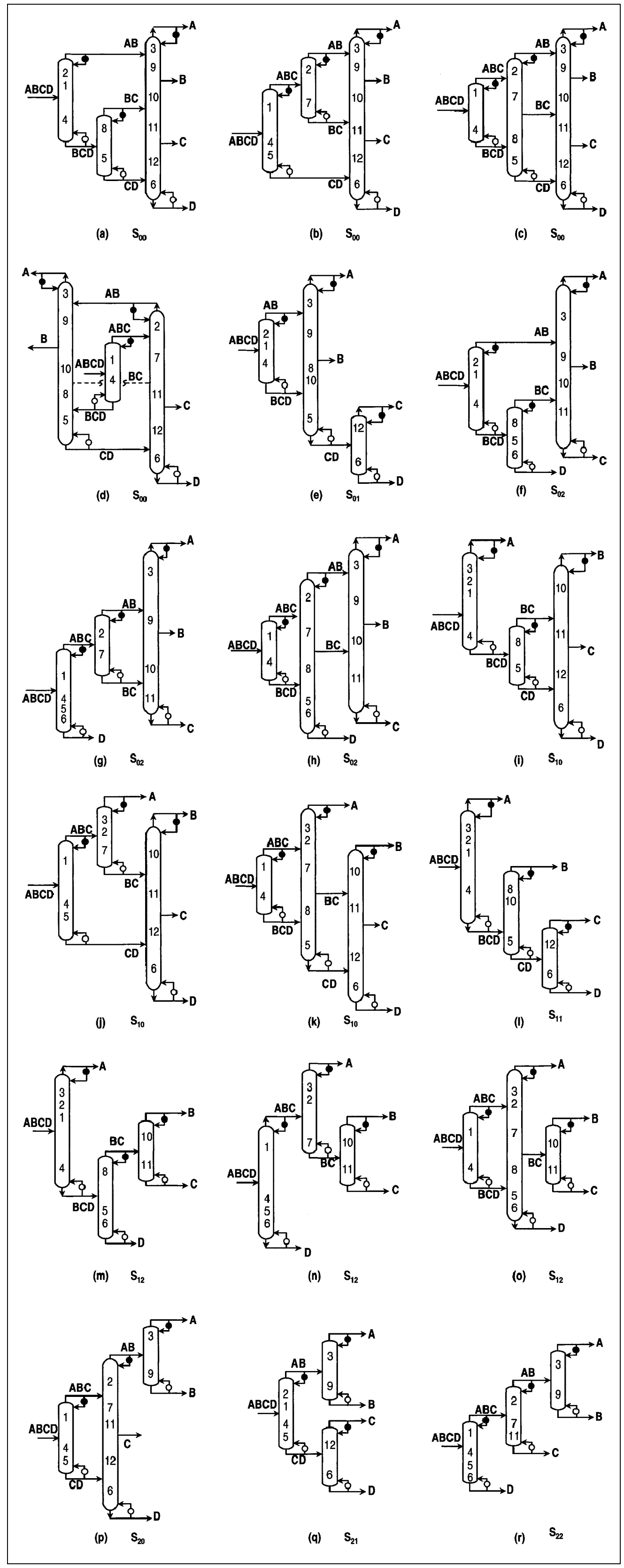

Figure 7. Basic configurations for a four-component distillation.

The first step will be to identify the heaviest intermediate product with an associated condenser and the lightest intermediate product with an associated reboiler. The heaviest intermediate product with an associated condenser is designated as the "heavy condenser component," and the lightest intermediate product stream with an associated reboiler is designated as the "light reboiler component." Now, one has a choice to initiate the modification of the n−component network either through the heavy condenser component or the light reboiler component. Either choice will lead to the same basic distillation configurations and, therefore, it is sufficient to follow only one of the two choices:

(i) First consider the choice where n−component network modification is initiated through the heavy condenser component using the steps described in case a. As observed from Figures 5c–5e, this will result in all other intermediate product streams that are more volatile than the heavy condenser component to be at a depth of $n-1$ in the modified network. When there is no other intermediate product stream heavier than the heavy condenser component that uses a reboiler, no further modification of the network is then needed. The modified network will provide the knowledge of the applicable $(n-1)$−component network options needed to identify possible configurations for the n−component mixture. For example, in option S_{21} a condenser is used with C and reboiler with B. Using the method outlined in case a, the original network is first modified through the heaviest intermediate product stream associated with a condenser. For the example problem, this leads to the modified network S_{01} in Figure 6b. Now at the depth of three, a reboiler is to be used with B. This leads to the distillation configuration of the ternary network option S_2 being applicable. The resulting configuration is shown in Figure 7q.

If there are intermediate products associated with reboilers that are heavier than the heavy condenser component, then, among such intermediate products, pick the one that is closest in volatility to the heavy condenser component, and further modify the network using the method described in case b. As observed from Figures 8c–8e, in the remodified network, all the product streams heavier than this intermediate product will now be located at the depth of $n-1$.

Therefore, after this remodification step, all other intermediate product streams with reboilers and condensers (except the heavy condenser component and its closest heavier component with a reboiler) will now be located at the depth of $n-1$. The remodified network is then used to create the appropriate distillation configurations. As an example consider option S_{12}. B is now the heavy condenser component, and the closest heavier component with a reboiler is C. Therefore, the network in Figure 3b is first modified according to the method in case a by eliminating submixtures containing B as the heaviest subgroup. The resulting modified network

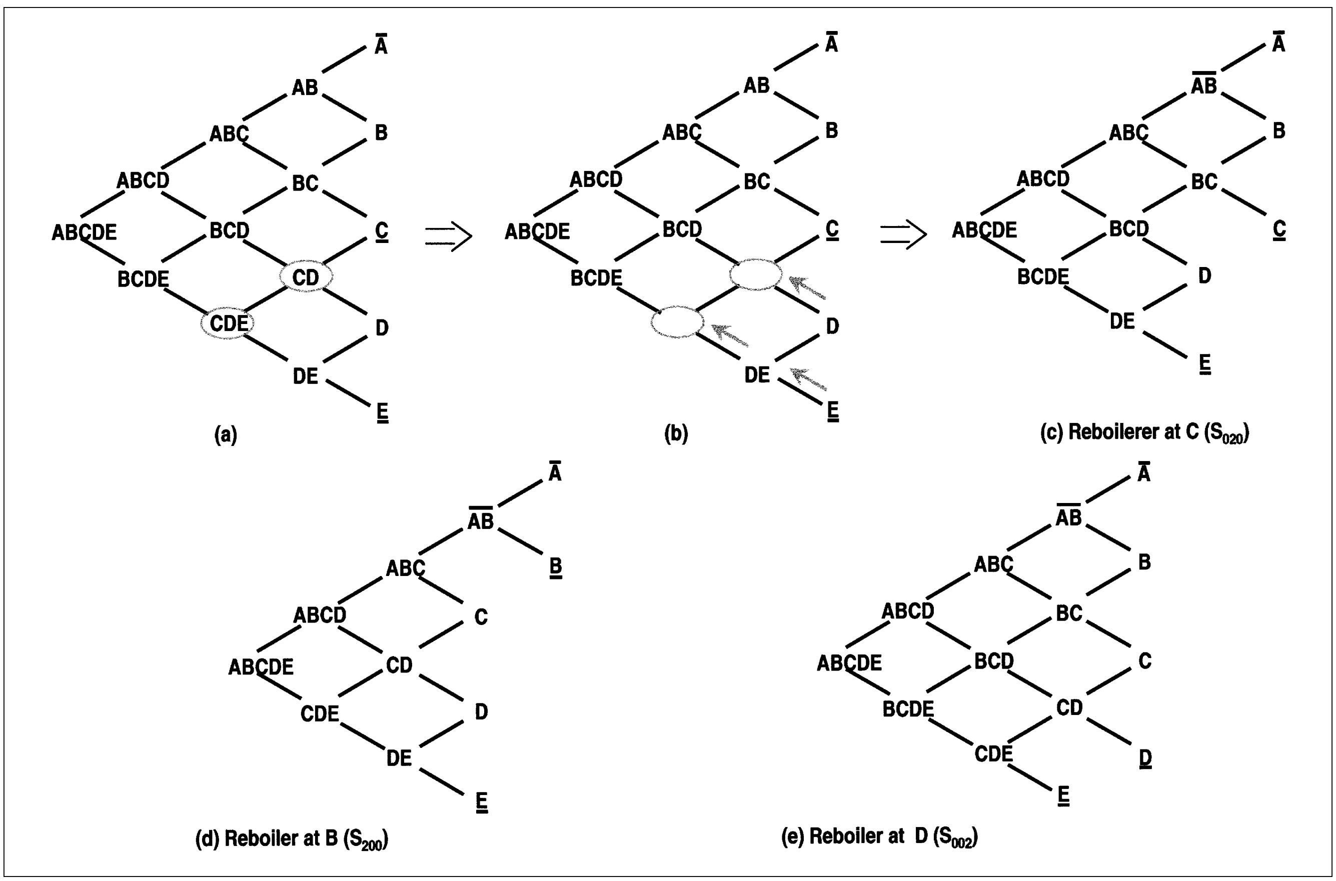

Figure 8. (a)–(c) Modification of a five-component network to eliminate submixtures *CD* and *CDE* in option S_{020}; modified networks for options (d) S_{200} and (e) S_{002}.

is S_{10}, shown in Figure 6a. Case b is then used with this modified network to provide the final modified network shown in Figure 6e. From the final network in Figure 6e, it is seen that the internal binary mixture BC at the depth of three has all three possible choices of reboilers and condensers available to it. This leads to distillation configuration of all the ternary network options (S_{ϕ}) being applicable. The resulting three configurations are shown in Figures 7m, 7n and 7o.

(ii) Alternatively the same distillation configurations can be generated by initiating the modification of the n−component network through the light reboiler component using the steps described in case b. In this alternative, the modified network will have all other intermediate product streams that are heavier than the light reboiler component at a depth of $n-1$. When there is no other intermediate product stream lighter than the light reboiler component that uses a condenser, then no further modification of the network is needed. The resulting configurations can be determined using applicable options for the $(n-1)$−component network. Let us now reconsider option S_{21}. This time, use the method of case b with the light reboiler component B to modify the original network. This will lead to the modified network S_{20} in Figure 6c. Now, a condenser is to be used in the modified network with component C at the depth of three, leading to the applicable distillation configuration of ternary network option S_1. Once again, the resulting configuration is shown in Figure 7q.

If there is at least one intermediate product stream with an associated condenser that is lighter than the light reboiler component, a subsequent modification of the network is then needed. In the modified network, choose the heaviest intermediate product among the intermediate product streams with associated condensers that are lighter than the light reboiler component and apply to it the method described in case a. Once again in the remodified network, all other intermediate product streams with reboilers and condensers (except the light reboiler component and its closest lighter component with a condenser) will now be located at the depth of $n-1$. The remodified network is then used to create applicable $(n-1)$−component network options. This method could easily be applied to the earlier option S_{12} for the four-component mixture to recreate a network in Figure 6e. However, for further illustration, consider option S_{121} for the five-component mixture $ABCDE$. Condensers are used here with each B and D, and a reboiler is used with C. The first modification with C as the light reboiler component results in the modified network of Figure 8c. Then, using B as the closest light component to C that has a condenser, submixture AB is eliminated from the resulting network, according to the method in case a. This leads to a remodified network with a condenser at D located at the depth of four, while both B and C remain at the original depth of five. Knowledge of the four-component network (applicable options $S_{\phi 1} = S_{01} + S_{11} + S_{21}$) can now be used to draw the resulting configurations.

Case f. Finally, consider the case when no reboiler or condenser is used with any of the intermediate product streams. For a four-component mixture, S_{00} is such an option. In such cases, the most straightforward situation is to retain all the binary submixtures at the depth of $n-1$ in the original network (Figure 3b). This is definitely a feasible solution because, from observation 6c, we know that the presence of all the binary submixtures in a network insures that all the intermediate products can be produced without need for a reboiler or condenser. In this solution, the binary mixture on the upper branch will use a condenser because the intermediate product B does not have a condenser (observations 6c and 5a). Similarly, the binary mixture on the lower branch has a reboiler associated with it (observations 6c and 5b). For other internal binary mixtures at the depth of $n-1$, all three possible choices of reboilers and condensers are available. This makes this solution equivalent to an $(n-1)$−component network problem with the same number of options and configurations. Therefore, this possible solution for S_{00} uses distillation configurations from all the ternary network options (S_{ϕ}). The resulting three configurations (corresponding to S_0, S_1, and S_2) are shown in Figures 7a, 7b, and 7c.

However, the solution cited above does not cover all possible configurations because observations 6c and 7 do not require that an internal submixture needed for the recovery of another internal submixture at the depth m be recovered at the depth of $m-1$. Whenever feasible, the internal submixture could be recovered at any suitable depth earlier than $m-1$. One such example for the S_{00} option for a four-component mixture is shown in Figure 6f. Intermediate products B and C use neither a reboiler, nor a condenser. It is seen from Figure 3b that the only submixture that has B as a heavy subgroup is AB. Therefore, it must be fed to the distillation section above the withdrawal location of B. However, both submixtures BC and BCD have B as a light subgroup. Therefore, both are candidates for providing boilup to the distillation section below the withdrawal location of B. Configurations using submixture BC for this purpose have already been created (Figures 7a, 7b and 7c). However, for this case, it is also possible to eliminate the submixture BC from the network and to feed submixture BCD to the distillation section below the withdrawal location of B. The resulting network is shown in Figure 6f and the distillation column configuration in Figure 7d. This is the satellite column arrangement discussed earlier by Agrawal (1996a). In Table 1, the applicable ternary options for S_{00} are listed as $S_{\phi} + S_3$. While the subscript ϕ takes on values of 0, 1 and 2 and refers to the absence or presence of a condenser or a reboiler at BC, the subscript 3 refers to the absence of submixture BC itself. The value of S_3 is one. S_{ϕ} represents all the options for a ternary mixture and has a value of three. Therefore, the number of configurations for option S_{00} is four ($S_{00} = 4$).

It should be noted that we have not yet identified any observation that will lead to networks such as the one in Figure 6f. The following observation will fulfill this need:

Observation No. 8. *For an n−component mixture, whenever in the final modified network (that is, after application of Step 1 and Step 2 cases a−f), an internal submixture at depth m (where $m < n$) has submixtures containing more than one component as its immediate neighbors at the height above and below (but at the same depth m), then the internal submixture can be eliminated from the network.* For the four-component problem with no reboiler and condenser at B or C, the initially modified network remains unchanged at the depth of three (Figure 3b). The immediate neighbors of internal submixture BC at the same depth of three are AB and CD. Since both AB and CD contain more than one component, according to this observation, it is possible to eliminate BC from the network, obtaining network 6f. On the other hand, the modified network in Figure 6d is an example where submixture *BC* cannot be eliminated because the neighbor below is *D*, which does not contain more than one component.

To further illustrate this observation, consider a five-component mixture. Clearly, for the option S_{000} with no reboiler or condenser at intermediate product streams, the immediate neighbors of both the internal binary mixtures *BC* and *CD* are binary mixtures (Figure 3c). This implies that configurations can be created by eliminating *BC*, *CD*, or both from the network. These modified networks are shown in Figures 9a, 9b, and 9c. Now for the five-component option S_{000}, all the applicable four-component network options are obtained by accounting all the networks in Figures 3c, 9a, 9b, and 9c. Therefore, for option S_{000}, the applicable four-component network options are designated as $S_{\phi_1\phi_2}$, where ϕ_1 refers to *BC* and ϕ_2 to *C*. Both ϕ_1 and ϕ_2 can take the values of 0, 1, 2, and 3, where 3 refer to the absence of the submixture. Therefore, the total number of applicable options at the depth of $n-1$ is $\sum_{\phi_1=0}^{3}\sum_{\phi_2=0}^{3} S_{\phi_1\phi_2}$. This can also be written as $S_{\phi\phi} + S_{3\phi} + S_{\phi 3} + S_{33}$, where subscript ϕ takes the values 0, 1, and 2. $S_{\phi\phi}$ refers to all possible four-component options, and includes all 18 distillation configurations derived for a four-component mixture. This means that each of the eighteen distillation configurations shown in Figure 7 can be used to produce binary mixtures *AB*, *BC*, *CD*, and *DE*, which are then fed to a distillation column to produce the product streams. $S_{3\phi}$ refers to options $S_{30} + S_{31} + S_{32}$, that is, in the network of Figure 9a all three possibilities with or without a reboiler or a condenser at *CD* are considered. If we consider S_{30} and look for the distillation configurations up to the depth of three, we find from observation 8 that two distinct possibilities exist. In one possibility, internal submixture *BCD* is transferred between the two distillation columns and we have three possible configurations of the first two distillation columns ($S_0 + S_1 + S_2$). The complete distillation column arrangements for these three possible configurations are shown in Figures 10a−10c respectively. In the second possibility, internal submixture *BCD* is eliminated and we have one configuration (S_3). The complete distillation column arrangement is shown in Figure 10d. While the arrangement of the first three distillation columns in any configuration of this figure is not identical to any of the four-component distillation configurations shown in Figure 7a through 7d, the num-

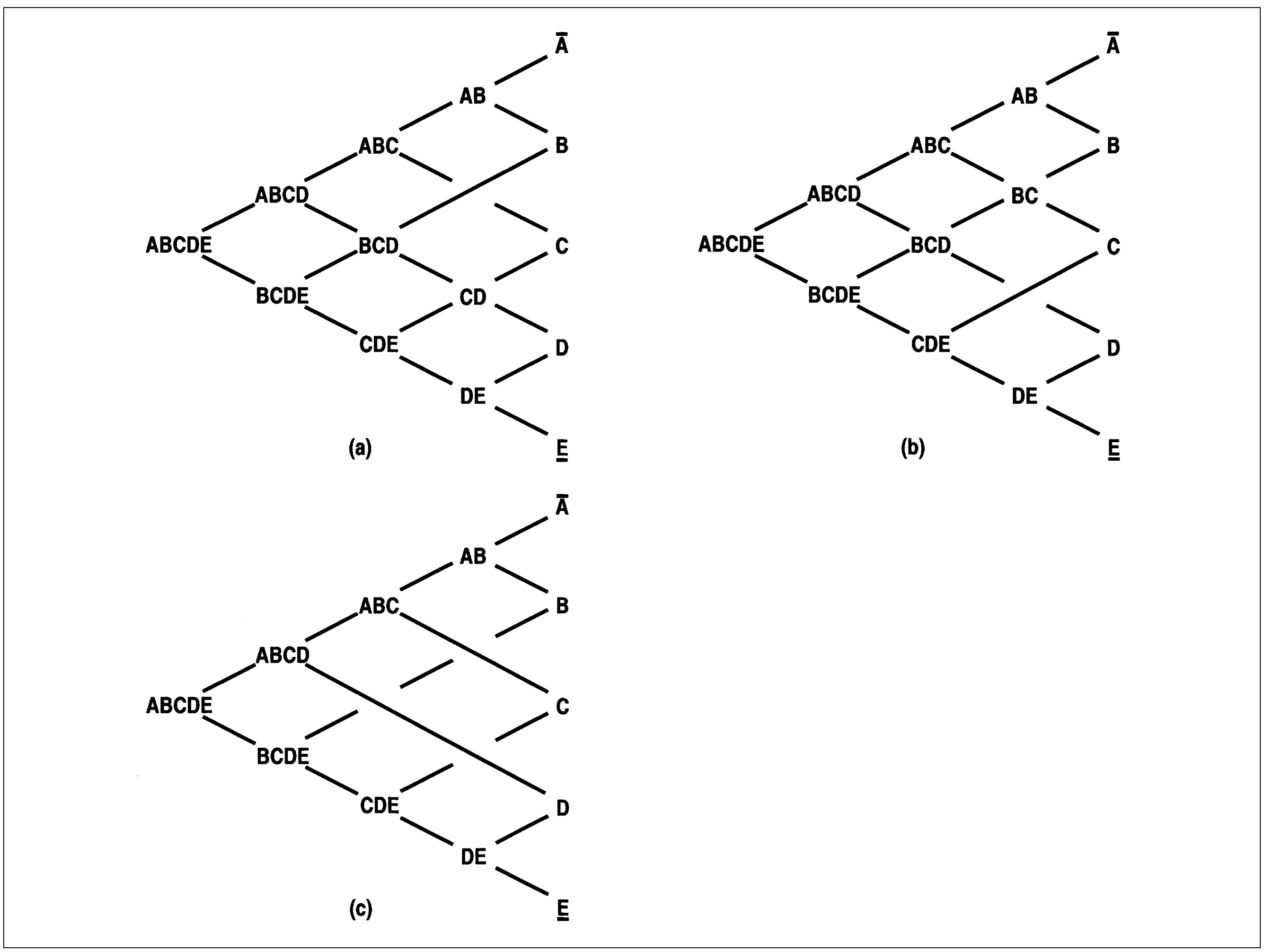

Figure 9. Possible networks for option S_{000} of a five-component mixture.

(a) Absence of *BC*, (b) absence of *CD*, (c) absence of both *BC* and *CD*.

ber of configurations for S_{30} is the same as for S_{00}. This follows from the fact that a further reduction of S_{30} and S_{00} leads to the same number of options up to the depth of three $(S_0 + S_1 + S_2 + S_3)$. Note that in the four-component network (Figure 3b), binary mixture AB located at the depth of three provides reflux for an internal submixture (B) at the next depth, and the binary mixture BC located below AB provides boilup for an internal submixture (B) at the next depth. An analogous situation exists for the network in Figure 9a. Here, the internal submixture ABC at the depth of three provides reflux for an internal submixture (C) located at a greater depth, and the internal submixture BCD located underneath ABC provides boilup for an internal submixture (B) that is also located at a greater depth. This leads to the next observation.

Observation No. 9. *When in a modified network, the applicable network option at the depth of $(n-1)$ is represented by an S with all the subscripts as 3, then there is only one configuration and that configuration is the satellite column arrangement.* This occurs when no reboiler or condenser is associated with the intermediate product streams and all the internal submixtures at the at the depth of $(n-1)$ have been eliminated. In the five-component S_{000} example, the applicable network option S_{33} at the depth of four in Figure 9c is such a case. *In all other options where 3 appears with other numbers (0, 1 or 2) as subscript in S, the number of possible configurations can be easily calculated by replacing every 3 with a zero and finding the number of configurations from the corresponding $(n-1)-$component network option.* Thus, in the five-component example, the number of configurations for option S_{31} at the depth of four in the modified network of Figure 9a is the same as for four-component option S_{01}, that is, only one configuration exists for this option (Table 1). Similarly, S_{32} has the same number of configurations as S_{02}; from Table 1, this number is three. Therefore, $S_{3\phi} = S_{30} + S_{31} + S_{32} = 4 + 1 + 3 = 8$. The value of $S_{\phi 3}(= S_{03} + S_{13} + S_{23} \Rightarrow S_{00} + S_{10} + S_{20})$ can be calculated with the help of Table 1 to be 8. This gives the value of S_{000} to be 35 $(S_{\phi\phi} + S_{3\phi} + S_{\phi 3} + S_{33} = 18 + 8 + 8 + 1 = 35)$. A word of caution is essential here. Just because the numeric value of S_{32} is equal to S_{02}, it does not mean that these five-component configurations are derived by simply adding a distillation column to each of the four-component configuration corresponding to S_{02}. This can be seen by comparing the five-component distillation configurations for

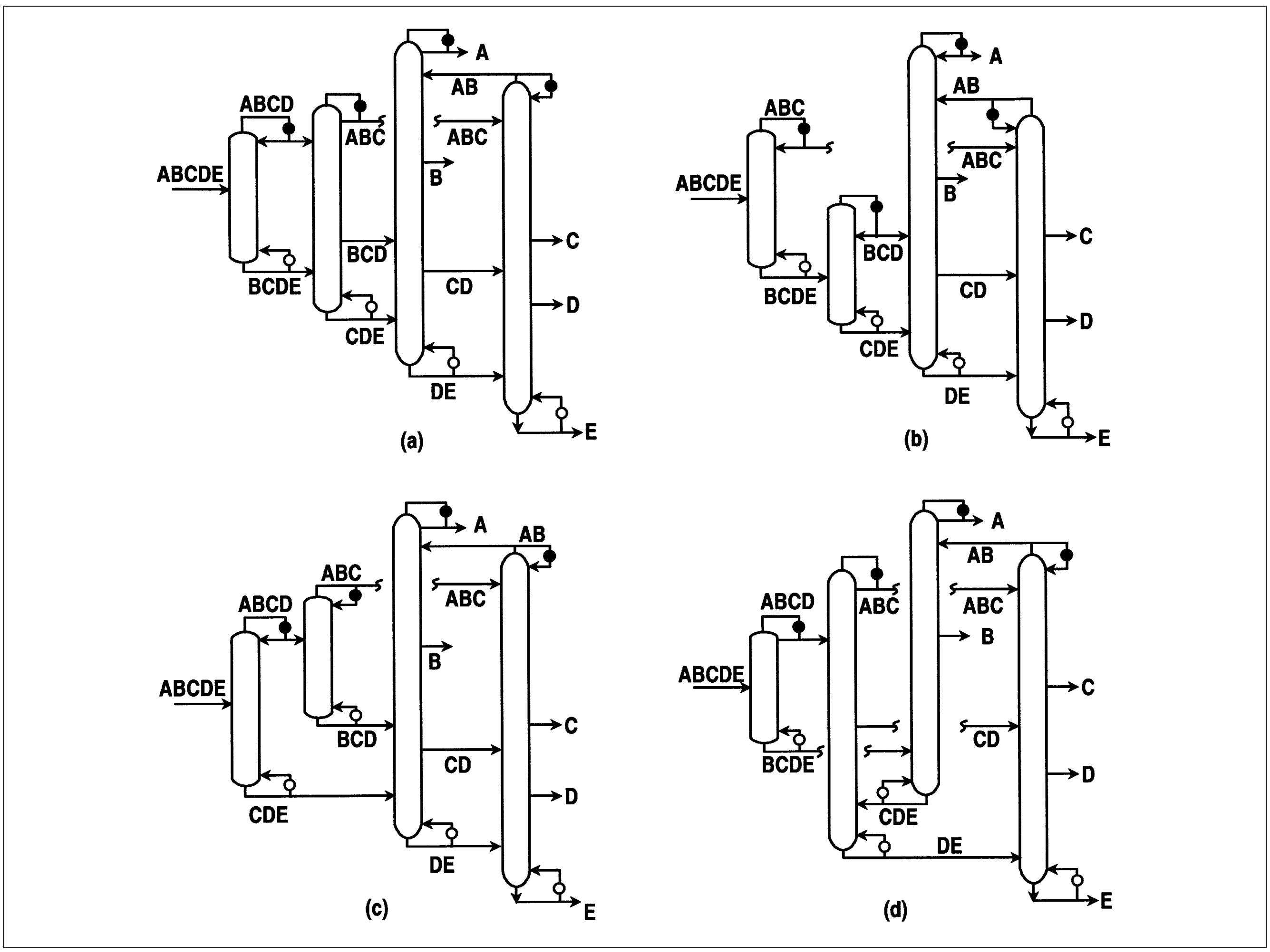

Figure 10. Five-component distillation configurations for case S_{000} without any inter-column transfer of submixture *BC*.

S_{30} in Figure 10 with the four-component configurations for S_{00} in Figures 7a through 7d.

A flow chart of the stepwise method is presented in Figure 11. This flow chart helps to visualize the procedure and can be used as an aid to draw basic distillation configurations for any given n-component mixture.

If needed, all the $n-1$ reboilers and $n-1$ condensers can be assigned by the proposed method to create a final network representation for any one specific configuration. This is done by first assigning the pre-specified reboilers and condensers to the intermediate product streams at the depth of n. Next, reboilers and condensers are assigned to the needed subgroups at the depth of $n-1$ in the modified network, and, then, by the application of the proposed method, the network is further modified to the equivalent $(n-2)$–component network problem. This procedure is continued by assigning reboilers and condensers to successive lower depths and each time modifying the network by the proposed method. The procedure is finished when all the reboilers and condensers are assigned. The final resulting network will represent a specific basic distillation configuration.

For a five-component mixture, all possible 27 $(=3^3)$ options are listed in Table 2. For this mixture, there are a total of 198 $(=S_{\phi\phi\phi})$ basic configurations. As expected, the total number of basic configurations increases rapidly as the number of components in a mixture is increased; a six-component mixture has 4,079 basic configurations!

In the proposed method, once reboilers and condensers have been assigned to the intermediate product streams, it is relatively easy to calculate the minimum, as well as maximum, number of distillation sections that could be present in the final basic distillation configurations. Whenever the values of the minimum and the maximum number of sections are different, more than one basic distillation configuration exists for the same assignment of reboilers and condensers to the intermediate product streams. A detailed discussion of this subject is presented in the Appendix.

Before concluding the development of a method to draw all possible basic configurations for an n–component mixture, it is useful to make one additional comment. In the configurations drawn according to observation 8, it may be possible to reintroduce the eliminated internal submixtures. For example, in the network representation of Figure 6f, binary submixture BC is eliminated. However, in the corresponding distillation column configuration of Figure 7d, there are two columns where binary mixtures of B and C exist. One such column is the one producing B and the other is the one producing C. In Figure 7d, two locations in these column sec-

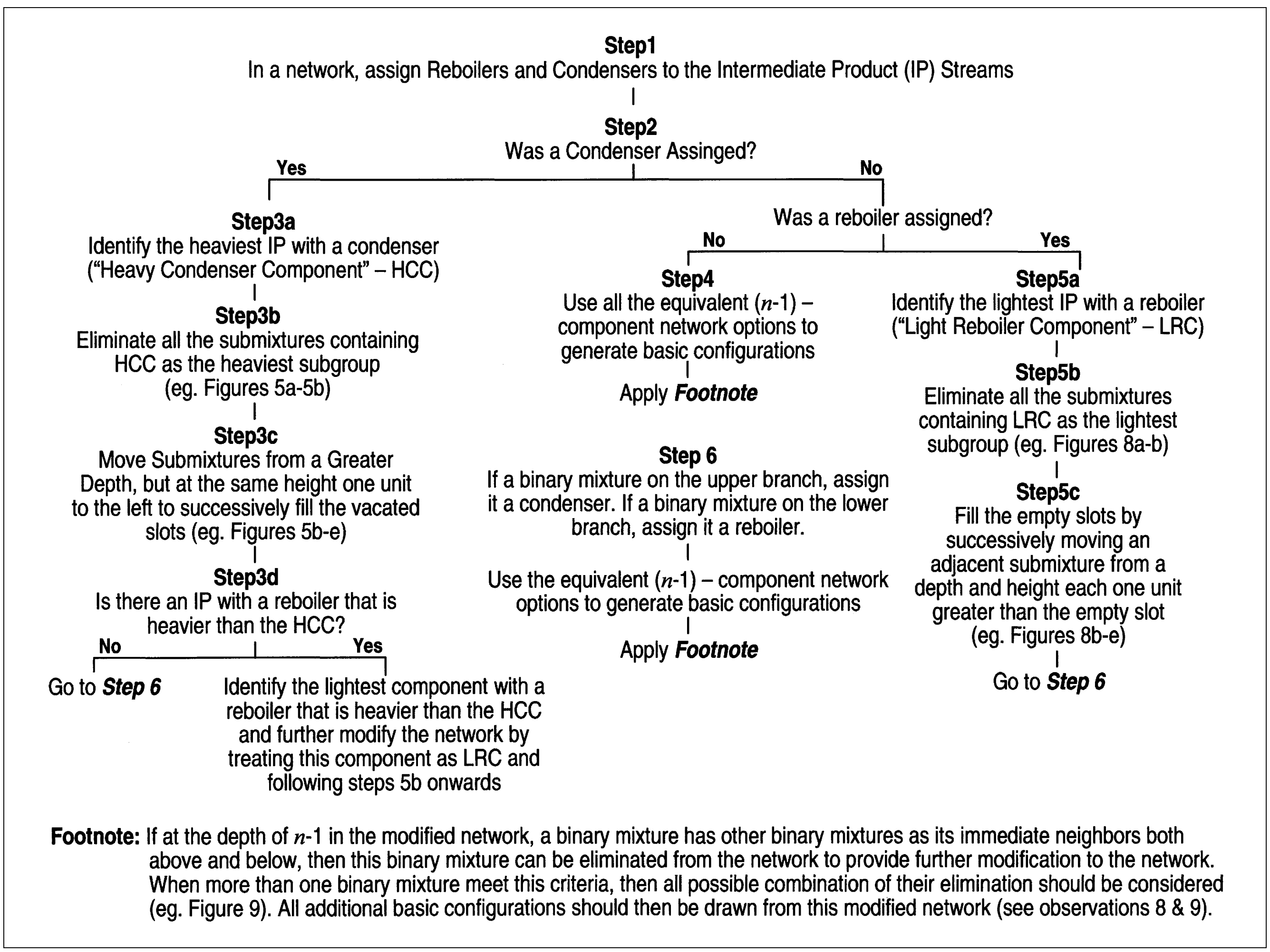

Figure 11. Stepwise procedure to draw basic distillation configurations from an n–component network.

Table 2. Basic Distillation Configuration Options for a Five-Component Mixture

Options	Shortcut	Applicable Quaternary Options	No. of Config. N_{BC}
S_{000}	$ABCDE \rightarrow \phi\phi\phi\phi$	$S_{\phi\phi} + S_{3\phi} + S_{\phi 3} + S_{33}$	35
S_{001}	$ABC\overline{D}E \rightarrow ABC\phi$	S_{00}	4
S_{002}	$ABC\underline{D}E \rightarrow \phi\phi\phi E$	$S_{\phi\phi} + S_{3\phi}$	26
S_{010}	$AB\overline{C}DE \rightarrow AB\phi\phi$	$S_{0\phi}$	8
S_{011}	$AB\overline{C}\overline{D}E \rightarrow AB\overline{C}\phi$	S_{01}	1
S_{012}	$AB\overline{C}\underline{D}E \rightarrow AB\phi E$	$S_{0\phi}$	8
S_{020}	$AB\underline{C}DE \rightarrow \phi\phi DE$	$S_{\phi 0}$	8
S_{021}	$AB\underline{C}\overline{D}E \rightarrow AB\underline{C}\phi$	S_{02}	3
S_{022}	$AB\underline{C}\underline{D}E \rightarrow \phi\phi\underline{D}E$	$S_{\phi 2}$	7
S_{100}	$A\overline{B}CDE \rightarrow A_{\phi\phi\phi}$	$S_{\phi\phi} + S_{\phi 3}$	26
S_{101}	$A\overline{B}C\overline{D}E \rightarrow A\overline{B}C\phi$	S_{10}	3
S_{102}	$A\overline{B}C\underline{D}E \rightarrow A\phi\phi E$	$S_{\phi\phi}$	18
S_{110}	$A\overline{B}\overline{C}DE \rightarrow A\overline{B}\phi\phi$	$S_{1\phi}$	7
S_{111}	$A\overline{B}\overline{C}\overline{D}E \rightarrow A\overline{B}\overline{C}\phi$	S_{11}	1
S_{112}	$A\overline{B}\overline{C}\underline{D}E \rightarrow A\overline{B}\phi E$	$S_{1\phi}$	7
S_{120}	$A\overline{B}\underline{C}DE \rightarrow A\phi DE$	$S_{\phi 0}$	8
S_{121}	$A\overline{B}\underline{C}\overline{D}E \rightarrow A\overline{B}\underline{C}\phi$	S_{12}	3
S_{122}	$A\overline{B}\underline{C}\underline{D}E \rightarrow A\phi\underline{D}E$	$S_{\phi 2}$	7
S_{200}	$A\underline{B}CDE \rightarrow \phi CDE$	S_{00}	4
S_{201}	$A\underline{B}C\overline{D}E \rightarrow \phi C\overline{D}E$	S_{01}	1
S_{202}	$A\underline{B}C\underline{D}E \rightarrow \phi C\underline{D}E$	S_{02}	3
S_{210}	$A\underline{B}\overline{C}DE \rightarrow \phi\overline{C}DE$	S_{10}	3
S_{211}	$A\underline{B}\overline{C}\overline{D}E \rightarrow \phi\overline{C}\overline{D}E$	S_{11}	1
S_{212}	$A\underline{B}\overline{C}\underline{D}E \rightarrow \phi\overline{C}\underline{D}E$	S_{12}	3
S_{220}	$A\underline{B}\underline{C}DE \rightarrow \phi\underline{C}DE$	S_{20}	1
S_{221}	$A\underline{B}\underline{C}\overline{D}E \rightarrow \phi\underline{C}\overline{D}E$	S_{21}	1
S_{222}	$A\underline{B}\underline{C}\underline{D}E \rightarrow \phi\underline{C}\underline{D}E$	S_{22}	1
			$S_{\phi\phi\phi} = 198$

tions are connected by a dotted line to signify that a binary mixture BC may be transferred between them. Similar connections can be drawn for the configurations in Figure 10. We have not yet investigated the advantage or disadvantage of such connections.

Now that the detailed description of the method to draw all of the basic configurations is complete, it is worthwhile to describe a shorter version of this method that can be used to reduce an n−component option to all the applicable $(n-1)$−component network options, but without having to draw any network representations.

Short version of the method for basic configurations

The method described so far basically assigns reboilers and condensers to the $(n-2)$ product streams of intermediate volatility and relates the n−component option to the options for an $(n-1)$−component mixture. This means that, after assigning reboilers and condensers at a depth of n in a network representation, the problem is translated to the assignment of reboilers and condensers at the depth of $(n-1)$. If needed, one could continue the process to the lower depths until all the reboilers and condensers up to the depth of two were assigned. This would lead to the creation of one specific configuration. However, with the information already available for the $(n-1)$−component mixture, there is generally no need to continue to the lower depths. The short version of the method that will be described in this section allows a quick translation of the given option from the depth of n to the options at the depth of $(n-1)$. The short method will now be illustrated in steps.

Step a. For an n−component mixture, each of the n components are located at the depth of n. They can be represented as a sequence of components; thus, for a five-component mixture, the sequence will be $ABCDE$. For any given option, the reboilers and condensers are then represented with overlines (for condensers) and underlines (for reboilers). For example, option S_{012} in Table 2 is represented as $AB\overline{C}\underline{D}E$. Recall that A always has a condenser and E a reboiler, so there is no need to show these in each sequence. In the following discussion, when we talk about reboilers and condensers associated with components, we talk only about product streams of intermediate volatility.

Step b. This step is only used if there is no intermediate product stream in the sequence with a reboiler that is heavier than the heaviest intermediate product with a condenser. Such an example is option S_{121} with sequence $A\overline{B}\underline{C}\overline{D}E$ in Table 2. Among the components of intermediate volatility, D is the heaviest component with a condenser and there is no other component of intermediate volatility with a reboiler to its right. The heaviest intermediate product with a condenser was earlier designated as the "heavy condenser component." In the sequence $A\overline{B}\underline{C}\overline{D}E$, $\overline{D}$, is the heavy condenser component. Now, in order to find the applicable $(n-1)$−component network options, the task is to reduce the number of members of the sequence from n to $n-1$. For this purpose, first write all of the components to the left of the heavy condenser component as present in the original sequence with their associated reboilers and condensers. For the sequence $A\overline{B}\underline{C}\overline{D}E$, it means writing $A\overline{B}\underline{C}$. Then, count the number of components to the right of the heavy condenser component in the original sequence and add the same number of ϕ's to the reduced sequence. In $A\overline{B}\underline{C}\overline{D}E$, there is only one component to the right of the heavy condenser component $\overline{D}$ so this leads to the reduced sequence $A\overline{B}\underline{C}\phi$ (for visualization see modified network of Figure 5e). A and ϕ can now be ignored and an associated condenser with B and a reboiler with C leads to equivalent option S_{12} for a four-component network. Thus, the five-component option S_{121} reduces to option S_{12} of a four-component network.

Let us consider another option S_{010} from Table 2. The corresponding original sequence is $AB\overline{C}DE$ with $\overline{C}$ as the heavy condenser component. The reduced sequence is $AB\phi\phi$, which leads to equivalent option $S_{0\phi}$ for a four-component network. Because the solution to the problem is initiated by specifying associated reboilers and condensers with only the intermediate product streams, each of the internal binary mixtures has a choice to use, or not to use, a reboiler or a condenser. Thus, ϕ takes on the values 0, 1, and 2. In this example problem, $S_{0\phi}$ refers to the options S_{00}, S_{01} and S_{02} of a four-component network.

A special case arises when, in the reduced sequence, a given ϕ has another ϕ as its neighbor on each side. In such situations, besides the three possibilities of having or not having a reboiler or a condenser, it is possible to eliminate the given ϕ (that is, internal binary mixture) from the final configuration (observation 8). As an example, consider option S_{100} for a five-component mixture in Table 2 (Figure 5d). The original sequence is $A\overline{B}CDE$ and the reduced sequence is $A\phi\phi\phi$. In the reduced sequence, the second ϕ from the left has a ϕ on each of its sides. Therefore, it has a choice to be present or absent from the final configuration. In order to acknowledge this choice, the equivalent four-component network options are written as $S_{\phi\phi_1}$, where ϕ_1 can take values of 0, 1, 2 and 3. $S_{\phi\phi_1}$ can also be written as $S_{\phi\phi} + S_{\phi 3}$, where ϕ only takes values 0, 1, and 2. While $S_{\phi\phi}$ includes all the nine options of a four-component mixture and yields 18 distillation column configurations, $S_{\phi 3}$ is equal to $S_{03} + S_{13} + S_{23}$. From the earlier discussion, we know that, when all the subscripts are not 3, they then can be treated as zero to calculate the number of possible distillation configurations. Thus, the number of configurations for $S_{\phi 3}$ is also equal to $S_{00} + S_{10} + S_{20}$, and, with the help of Table 1, this turns out to be 8 distillation configurations. Therefore, the total number of distillation configurations corresponding to option S_{100} for a five-component mixture is 26.

Application of Step b is particularly attractive when, in a given option, the heaviest intermediate product stream has a condenser. The $n-$component option then reduces to the corresponding $(n-1)-$component network option by simply eliminating 1 from the last subscript in S. In one of the examples discussed earlier, option S_{121} for a five-component mixture translated into S_{12}. Similarly in Table 2, S_{001}, S_{011}, S_{021} —S_{221} translate into S_{00}, S_{01}, S_{02}—S_{22}.

It is worth noting that in this shortcut method, the reduced sequence uses ϕ for any of the binary mixture present at the depth of $n-1$ in the modified network. However, if needed, the information is available to identify each of the binary mixtures present in the reduced sequence. A ϕ in the first slot of the reduced sequence represents binary mixture AB, a ϕ in the second slot represents BC and so on. As an example, consider option S_{10} for a four-component mixture. The corresponding reduced sequence is $A\phi\phi$ (Table 1) and the modified network is shown in Figure 6a. Since the first ϕ is in the second slot, it represents binary mixture BC and the next ϕ represents CD.

Step c. This step is only used, if in the original sequence, there is no intermediate product stream with a condenser that is lighter than the lightest intermediate product stream with a reboiler. The lightest intermediate product with a reboiler was earlier designated as a "light reboiler component." The reduced sequence is generated by first writing a ϕ for each component that is to the left of the light reboiler component. Then, the exact subsequence from the right of the light reboiler component in the original sequence is added to the reduced sequence. For example, consider option S_{021} for a five-component mixture. The original sequence is $AB\underline{C}\overline{D}E$ and $\underline{C}$ is the light reboiler component. There are two components that are to the left of $\underline{C}$ and, as a result, the reduced sequence starts with two ϕs. The subsequence $\overline{D}E$ from the right of $\underline{C}$ is then added to complete the reduced sequence. This leads to a reduced sequence $\phi\phi\overline{D}E$ (for visualization see modified network in Figure 8c). This corresponds to options contained in $S_{\phi 1}$ for a four-component network. Since $S_{\phi 1} = S_{01} + S_{11} + S_{21}$, a total of three distillation configurations are obtained for this option from Table 1. Note that one could alternatively use Step b with this option S_{021} in Table 2 and arrive at the same result.

Once again, when in the reduced sequence, a given ϕ has another ϕ as its neighbor on each side, this then leads to another possibility whereby distillation configurations can be created without using this ϕ (and the corresponding internal binary mixture). One must account for this possibility as described in Step b. As an example, consider option S_{002} for a five-component mixture in Table 2. The original sequence is $ABC\underline{D}E$ and the corresponding reduced sequence is $\phi\phi\phi E$. This leads to options contained in $S_{\phi_1\phi}$ of a four-component network. $S_{\phi_1\phi}$ is equal to $S_{\phi\phi} + S_{3\phi}$ and the number of distillation configurations contained in $S_{3\phi}$ is equal to $S_{00} + S_{01} + S_{02}$ (corresponding to $S_{30} + S_{31} + S_{32}$). For the option S_{002}, this leads to a total of 26 distillation configurations from Table 1.

As expected, application of the Step c is particularly attractive when, in a given option, the lightest intermediate product stream has a reboiler. For this case, the $n-$component option is reduced to corresponding $(n-1)-$component network option by simply eliminating 2 from the first subscript in S. Therefore, in Table 2, options S_{200}, S_{201}, —S_{222} translate into the equivalent four-component network options S_{00},S_{01}, —S_{22}.

Step d. This step is to be used when conditions in the earlier steps b and c are not satisfied. Now there are two possibilities: (1) at least one intermediate component that is heavier than the heavy condenser component has a reboiler, or (2) at least one intermediate component that is lighter than the light reboiler component has a condenser.

First consider the possibility when at least one intermediate component is heavier than the heavy condenser component and has a reboiler. As an example, consider option S_{0102} for a six-component mixture. The original sequence is $AB\overline{C}D\underline{E}F$ with $\overline{C}$ as the heavy condenser component. The first portion of the reduced sequence is now written in accordance with Step b, that is, the subsequence to the left of the heavy condenser component in the original sequence is reproduced in the reduced sequence. The closest intermediate component to the right of the heavy condenser component that has a reboiler is then identified ($\underline{E}$). For every component between these two components, plus one additional ϕ is then added to the reduced sequence. Finally, the reduced sequence is completed by reproducing the subsequence from the right of the identified closest reboiler-containing component that is to the right of the heavy condenser component. In the example option, therefore, the reduced sequence starts with AB. Then two ϕ's are added (one for D between $\overline{C}$ and $\underline{E}$, plus an additional one). The reduced sequence is completed by adding the subsequence to the right of $\underline{E}$. The completed reduced sequence is $AB\phi\phi F$ with the equivalent option $S_{0\phi\phi}$ for a five-component network.

The second possibility, when at least one intermediate component lighter than the light reboiler component has a condenser, can be similarly described. First, the intermediate component with a condenser that is closest to the light reboiler component and is to the left of it in the sequence (that is, the heaviest intermediate component with a condenser that is lighter than the light reboiler component) is identified. Next, the subsequence to the left of this component is reproduced in the reduced sequence. Then, for every component between the identified component and the light reboiler component, plus an additional ϕ is added to the reduced sequence. The reduced sequence is then completed by adding the subsequence to the right of the light reboiler component in the original sequence. As an example, consider option S_{1122}

for a six-component mixture. The original sequence is $A\bar{B}\bar{C}\underline{\underline{D}}\underline{E}F$. In this example, $\underline{D}$ is the light reboiler component and $\bar{\bar{C}}$ is the closest intermediate component on the left of $\underline{D}$ that has a condenser. Therefore, $A\bar{B}$ followed by one ϕ (no component between $\bar{C}$ and $\underline{D}$) and then $\underline{E}F$ forms the reduced sequence $A\bar{B}\phi\underline{E}F$. This leads to the equivalent option $S_{1\phi 2}(=S_{102}+S_{112}+S_{122})$ for a five-component network. From Table 2, it is apparent that option S_{1122} has 32 basic distillation configurations.

For both of these possibilities, if a ϕ in the reduced sequence has any other ϕ as its neighbor on each of its sides, then the alternative of not using this ϕ in the final distillation configuration must be accounted for. This is similar to the action taken previously for steps b and c. For example, consider option S_{1002} for a six-component mixture. The original sequence is $A\bar{B}CD\underline{E}F$ and the reduced sequence is $A\phi\phi\phi F$. The corresponding five-component network option is written as $S_{\phi\phi_1\phi}$, where ϕ_1 takes an additional value of 3. For a five-component network, $S_{\phi\phi_1\phi}=S_{\phi\phi\phi}+S_{\phi 3\phi}$, and the number of configurations for $S_{\phi 3\phi}$ are the same as for $S_{\phi 0\phi}$. From Table 2, $S_{\phi\phi\phi}=198$ and $S_{\phi 0\phi}$ is calculated to be 120 from $\sum_{i=0}^{2}\sum_{j=0}^{2} S_{i0j}$ and Table 2. The total number of basic distillation configurations for S_{1002} is 318.

Step e. This step is used when no reboilers or condensers are used with the intermediate product streams. The reduced sequence has only ϕ's as its elements and their number is one less than the number of components in the original sequence. Thus, for a six-component mixture and option S_{0000}, the reduced sequence is $\phi\phi\phi\phi\phi$. Clearly all three ϕ's in the middle of the reduced sequence have another ϕ as its neighbor on each side and, therefore, distillation configurations can be created without them. This leads to equivalent five-component option $S_{\phi_1\phi_1\phi_1}$. Now $S_{\phi_1\phi_1\phi_1}=\sum_{i=0}^{3}\sum_{j=0}^{3}\sum_{k=0}^{3} S_{ijk}$, or $S_{\phi_1\phi_1\phi_1}=S_{\phi\phi\phi}+S_{3\phi\phi}+S_{\phi 3\phi}+S_{\phi\phi 3}+S_{33\phi}+S_{3\phi 3}+S_{\phi 33}+S_{333}$ with ϕ taking values 0, 1, and 2. In order to calculate the number of distillation configurations, every 3 that appears in the subscripts of S can be replaced with a 0 except in S_{333}. The number of configurations in $S_{333}\neq S_{000}$ and S_{333} contains only one satellite column configuration. The values of the rest of the options contained in $S_{\phi_1\phi_1\phi_1}$ are readily calculated with the aid of Table 2, and it is found that this option contains 700 basic distillation configurations.

Now that we know how to draw all possible basic distillation configurations for an n−component mixture, some comments can be made regarding the number of configurations for the different options.

Comments on the number of basic configurations

We have calculated that the numbers of basic distillation configurations for three, four, five and six-component mixtures are 3, 18, 198, and 4,079, respectively. Clearly, the number of basic distillation configurations rises rapidly as the number of components in the feed mixture increases. For a given n−component mixture ($n>3$), just one option where no reboiler or condenser is used with any of the intermediate product streams yields many more distillation configurations than for the $(n-1)$−component mixture. Some other interesting observations can also be made:

(i) For an n−component mixture, the number of options when the heaviest intermediate product stream uses a condenser is 3^{n-3}. From Step b of the short method described above, we know that this number of options is not only equal to the number of options for the $(n-1)$−component mixture, but it also contains the same number of basic distillation configurations. Thus, one-third of the total options contain the same number of distillation configurations as does the $(n-1)$−component mixture. By symmetry, the same is true for the one-third of the total options that contain a reboiler associated with the lightest intermediate product stream.

(ii) It does not follow from the above observations that two-thirds of the options contain twice as many basic distillation configurations as for an $(n-1)$−component mixture. The reason is that each subset of one-third options contains some common options where, simultaneously, a reboiler is present at the lightest intermediate product stream and a condenser is present at the heaviest intermediate product stream. The total number of such options is, in fact, 3^{n-4}. Therefore, the numbers of options that contain at least a reboiler at the lightest intermediate product stream or a condenser at the heaviest intermediate product stream are $2\times 3^{n-3}-3^{n-4}$ for all $n\geq 4$. This corresponds to 5/9th of the total options. It is possible to calculate the number of distillation configurations for the 3^{n-4} options. To do this, Step b of the short method is applied first, and then Step c is applied to the resulting reduced sequence. From the final reduced sequence, it is observed that this problem is similar to an $(n-2)$−component network problem. Therefore, these 3^{n-4} options have the same number of basic distillation configurations as does an $(n-2)$−component mixture. Thus, for an n−component mixture, the 5/9th of the options have $2\Psi_{n-1}-\Psi_{n-2}$ basic distillation configurations, where Ψ refers to the total number of basic configurations and the subscript refers to the number of components in the given mixture.

(iii) It is clear that sharp increase in the number of distillation configurations results from the other 4/9th of the total options that do not include an associated condenser with the heaviest intermediate product stream or a reboiler with the lightest intermediate product stream. The option that contains the greatest number of distillation column configurations is the one with no reboiler or condenser associated with any of the intermediate product streams. (This is true for $n>3$.) Thus, $S_{00}=4$, $S_{000}=35$ and $S_{0000}=700$. (It is interesting to compare them with $\Psi_3=3$, $\Psi_4=18$ and $\Psi_5=198$.) The next highest number of basic distillation configurations is for those options when only one condenser or one reboiler is used with the intermediate product streams, with the constraint that the condenser be used with the lightest intermediate product stream or the reboiler with the heaviest intermediate product stream. Thus, in Table 2, options S_{100} and S_{002} have the next highest number of distillation configurations. The number of distillation configurations declines rapidly as the single condenser is used with intermediate product streams of decreased volatility (compare S_{100}, S_{010}, and S_{001} in Table 2). The same is true as the single reboiler is used with intermediate product streams of increased volatility (options S_{002}, S_{020} and S_{200}). Similarly, as the number of reboilers and condensers associated with the intermediate product streams increases, the number of possible distillation configurations declines rapidly. In summary, a greater number of distillation configurations results for options where fewer condensers are used with the more volatile components and fewer reboilers are used with the heavier components.

(iv) It is observed from Tables 1 and 2 that certain options have equal numbers of distillation configurations. For example, in Table 2 the number of distillation configurations for S_{001} is equal to those for S_{200}, $S_{011} = S_{220}$, $S_{012} = S_{120}$, and so on. It is easy to identify situations when this is applicable through an inspection of modified networks such as the ones in Figure 6. For an n−component mixture, there are $n-2$ subscript digits associated with S. Each digit refers to a slot where a reboiler or a condenser could be placed. From a given option, another option is created by replacing a reboiler at the jth slot with a condenser at $(n-1)-j$ slot, and a condenser at the ith slot with a reboiler at $(n-1)-i$ slot. Similarly, empty slots transfer as empty slots. The created option will have the same number of basic distillation configurations as the original configuration. For a five-component mixture, $(n-1)-j = 4-j$ and consider option S_{012}. An option is created by replacing a reboiler in the third slot with a condenser in the first slot, a condenser in the second slot with a reboiler in the second slot, and the zero in the first slot with a zero in the third slot. This will be option S_{120} that has the same number of distillation configurations as S_{012}. Sometimes, the created option is identical to the original option. One such example in Table 2 is S_{102}. For a four-component mixture in Table 1, S_{12} and S_{21} are such examples.

(v) Multicomponent distillation configurations with sharp splits between components of adjacent volatilities in each distillation column are well known. Thompson and King (1972) presented an equation to calculate the number of such possible sequences for the separation of an n−component mixture into single-component product streams. The direct and indirect split configurations in Figure 1 are examples of sharp split configurations. The five known sharp split configurations for a four-component mixture are shown in Figures 7l, 7m, 7n, 7q, and 7r. It is readily observed that sharp split configurations result only for those options where each of the intermediate product streams either has a reboiler or a condenser associated with it. For a four-component mixture, it means that sharp split configurations are obtained from options S_{11}, S_{12}, S_{21} and S_{22}. Some of these options can have additional configurations that contain nonsharp separations. S_{12} is such an option—besides the two sharp split configurations shown in Figures 7m and 7n, it also leads to a configuration in Figure 7o that uses a nonsharp separation in the first column.

Thermally Coupled Distillation Configurations

Once the basic distillation configurations for an n−component mixture are known, it is easy to draw the corresponding distinct thermally coupled configurations associated with each one. It was discussed earlier that each of the known thermally coupled configurations for a ternary mixture shown in Figure 2 could be derived from the basic configurations shown in Figure 1. This was done by replacing the reboiler or condenser associated with a mixture with a two-way communication. This technique was earlier described to create thermally coupled configurations from the sharp split configurations of any n−component mixture (Agrawal, 1996a). We will now use the same method to generate all the distinct thermally coupled configurations from all the basic configurations. For a given n−component mixture, $n-1$ reboilers and $n-1$ condensers are used in any basic configuration. One of the condensers is assigned to the most volatile component and one reboiler to the heaviest component. This leaves $n-2$ reboilers and $n-2$ condensers. For any given option, we know the exact number of reboilers and condensers that are assigned to the intermediate product streams at depth n in a network. By difference, we then know the number of reboilers and condensers that are assigned to mixtures located at depths $n-1$ or earlier in a network. One or more of such reboilers and condensers can then be exchanged for two-way communications to create distinct thermally coupled configurations. In other words, distinct thermally coupled configurations, rather than basic configurations, can be generated by using a two-way communication in place of a reboiler or a condenser in the synthesis steps that were described earlier for the basic configurations. Replacing a mixture reboiler with a two-way communication leads to side rectifier-type of configurations, and replacing a mixture condenser with a two-way communication provides side stripper-type configurations. When all of the mixture reboilers and condensers are replaced with two-way communications, and none of the intermediate product streams has a reboiler or a condenser, then the resulting thermally coupled configuration has only one reboiler and one condenser. In these configurations, the total number of distillation sections vary from $4n-6$ to $n(n-1)$ (Agrawal, 1996a; also see the Appendix). Such thermally coupled configurations are called "fully-coupled" *only* when they contain a full set of $n(n-1)$ distillation sections.

Now it is easy to calculate the total number of distinct thermally coupled configurations for an n−component mixture. For a given basic configuration, let r and c be the respective numbers of reboilers and condensers associated with mixtures. Then, the number of distinct thermally coupled

Table 3. Distinct Thermally Coupled Configurations for a Four-Component Mixture

Option	N_{BC}	r	t_r	$T_r = N_{BC} \cdot t_r$	c	t_c	$T_c = N_{BC} \cdot t_c$	$t_m = t_r \cdot t_c$	$T_m = N_{BC} t_m$	$t_t = t_r + t_c + t_m$	$T_t = T_r + T_c + T_m$
S_{00}	4	2	3	12	2	3	12	9	36	15	60
S_{01}	1	2	3	3	1	1	1	3	3	7	7
S_{02}	3	1	1	3	2	3	9	3	9	7	21
S_{10}	3	2	3	9	1	1	3	3	9	7	21
S_{11}	1	2	3	3	0	0	0	0	0	3	3
S_{12}	3	1	1	3	1	1	3	1	3	3	9
S_{20}	1	1	1	1	2	3	3	3	3	7	7
S_{21}	1	1	1	1	1	1	1	1	1	3	3
S_{22}	1	0	0	0	2	3	3	0	0	3	3
Total:				$N_{TR} = 35$			$N_{TC} = 35$		$N_{TM} = 64$		$N_{TT} = 134$

configurations t_r, created when one or more of the r reboilers are replaced with a two-way communication, is equal to

$$\sum_{i=1}^{r} {}^{r}C_i$$

where ${}^{r}C_i = r!/i!(r-i)!$. Similarly, the number of distinct thermally coupled configurations t_c, when one or more of the c condensers are replaced with a two-way communication, is equal to

$$\sum_{i=l}^{c} {}^{c}C_i$$

Now the number of distinct thermally coupled configurations t_m, where at least one reboiler from the r reboilers and at least one condenser from the c condensers are replaced with two-way communications, is equal to $t_r \cdot t_c$. For a four-component mixture, the values of t_r, t_c, and t_m are given in Table 3. For any given option the total number of basic configurations N_{BC} can be read from Table 1. Then, the total number of distinct thermally coupled configurations for this option can be calculated from t_r, t_c, and t_m. For example, option S_{00} has four basic distillation configurations. For every basic configuration, it is possible to have three distinct thermally coupled configurations where one or more mixture reboiler is replaced with a two-way communication, but none of the condensers are replaced ($t_r = 3$). Therefore, the total number of such thermally coupled configurations for this option T_r is 12. Similarly, the total number of distinct thermally coupled configurations where only mixture condensers are replaced with two-way communications T_c is also 12. The total number of distinct thermally coupled configurations where both condensers and reboilers are replaced with two-way communications T_m, is $4 \times 3 \times 3 = 36$. The total number of distinct thermally coupled configurations for option S_{00}, T_t, is $4 \times (3 + 3 + 3 \times 3) = 60$. Considering all the options, there are a total of 134 distinct thermally coupled configurations for a four-component mixture in Table 3.

Similar calculations for a five-component mixture yields a total of 5,674 distinct thermally coupled configurations. 1,774 of these configurations involve cases where only mixture reboilers or mixture condensers are replaced with two-way communications. The remaining 3,900 cases involve the replacement of both reboilers and condensers.

For a four-component mixture, four distinct thermally coupled configurations each with only one condenser and one reboiler are shown in Figure 12. These were derived by replacing all of the mixture reboilers and condensers from the basic configurations corresponding to option S_{00} in Figures 7a through 7d. Each of the structures shown in Figure 12 is unique. In Figure 12d, the optional BC transfer of Figure 7d is not used in order to insure that structures in Figures 12c and 12d are different. Note that each of the configurations in Figures 12a, 12b and 12d uses ten distillation sections ($4n-6$), whereas the one in Figure 12c uses twelve ($n(n-1) = 12$). Thus, the configuration in Figure 12c suggested by Sargent and Gaminibandara (1976) is the only fully-coupled configuration. Whereas, the other three configurations in Figure 12, including the satellite configuration in Figure 12d, are not fully coupled configurations.

It is important to note that for each distinct thermally coupled configuration, corresponding thermodynamically equivalent configurations can be easily drawn by rearranging distillation sections to appropriate distillation columns (Agrawal, 1999, 2000b). For example, it is known that there are 32 thermodynamically equivalent configurations for the fully coupled configuration of Figure 12c (31 additional configurations besides the one shown in Figure 12c). Similarly, for each of the distinct thermally coupled configurations in Figures 12a, 12b and 12d, there are 15 additional thermodynamically equivalent configurations (a total of 16 thermodynamically equivalent configurations for each). These thermodynamically equivalent configurations are obtained due to the fact that conversion of each one-way communication in the basic distillation configuration to a two-way communication results in one additional possibility. For example, the elimination of condenser AB in Figure 7a leads to the two-way communication for AB in Figure 12a with the added possibility that distillation section 3 with the associated condenser could be located above the distillation section 2. Similarly, in this figure, distillation section 10 has a choice to be either on top of distillation section 11 or 8; distillation section 5 could be moved below distillation section 4; and distillation section 6 along with its reboiler could be moved below distillation section 5. Note that distillation sections 9 and 10, and also 11 and 12, must stay together (Step 1 of Agrawal, 2000b). All these additional possibilities result in 16 thermodynamically equivalent configurations for Figure 12a. Similarly, in the fully-coupled configuration Figure 12c, one additional possibility exists for the transfer of binary mixture BC. Distillation section 7 could be located above distillation section 11 with the simultaneous movement of distillation section 8 under distillation section 10. This provides a total of two possibilities for the transfer of binary mixture BC (Step 3 of Agrawal, 2000b). Therefore, one additional possibility exists for each two-way communication within the fully-coupled configuration and results in a total of 32 thermodynamically equivalent configurations.

For the pinched columns, the total vapor flow of a distinct thermally coupled configuration will be at its minimum and all of its thermodynamically equivalent configurations will have the same minimum vapor flow. Therefore, during a search for the optimum configuration, the search space of feasible distillation configurations could be reduced by excluding the thermodynamically equivalent configurations. This will limit the search space to the basic and distinct thermally coupled configurations.

In the synthesis method described above, no attention was paid to whether a generated distinct thermally coupled configuration is easily operable or not. If a distinct thermally coupled configuration is found to be economically optimum, but difficult to operate, its equivalent more operable structure can always be easily drawn (Agrawal, 1999; Agrawal and Fidkowski, 1999a). This technique modifies a thermally coupled configuration such that all the vapor streams flow from a higher pressure to a lower pressure. Consequently, no compressors are needed for such transfers. More operable configurations for the fully thermally coupled configuration in Figure 12c can be found elsewhere (Figures 3 and 4 of Agrawal, 1999).

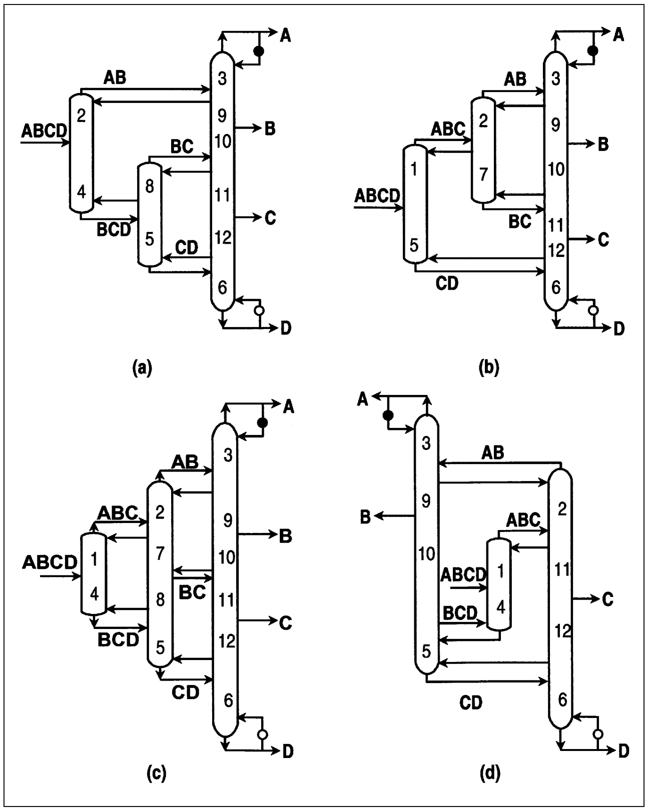

Figure 12. Thermally coupled configurations with only one reboiler and one condenser for a four-component mixture.

One final comment regarding the method for the synthesis of distinct thermally coupled configurations from the basic configurations. In some of the basic configurations, internal submixtures are withdrawn from an intermediate location of a distillation column and transferred to another distillation column. There is no reboiler or condenser associated with such a transfer of internal submixtures. Transfer of binary mixture *BC* in Figure 7c is an example of such a configuration. In this work we have not explored the possibility of having such transfers occur as two-way communications in the basic configuration itself, whereas we have considered this possibility in thermally coupled configurations. Thus, in Figure 12c, the distinct thermally coupled configuration derived from Figure 7c, shows the transfer of *BC* as a two-way communication. The use of a two-way communication for the transfer of an internal submixture allows the possibility of converting it to a one-way communication during an optimization process. Thus, an optimization procedure could determine the optimum flows for each stream and, if one of them is relatively small, it could then be turned off, resulting in a one-way communication. Therefore, in this work, all internal submixture transfers between the columns that do not have associated reboilers or condensers in the basic configurations are converted to a two-way communication to generate distinct thermally coupled configurations.

Miscellaneous Distillation Configurations

There are numerous other multicomponent distillation configurations that are not included in the basic and thermally coupled configurations just described. However, most of the known variations can easily be incorporated, as described below.

(i) In the derivation of basic configurations when a submixture is transferred from one distillation column to another, the thermodynamic state of the stream was not specified. Generally, one chooses this stream to be a saturated liquid or a saturated vapor. Thus, in Figure 7a, binary mixture *AB* can be transferred as a vapor (as shown in the figure) or a liquid stream from the condenser. The same is true for submixtures exiting a reboiler, such as *BCD*. The choice will generally depend on the specific application at hand. If thermodynamic efficiency is important, then submixtures from the tops of columns, such as binary mixture *AB*, are transferred as vapor streams, and submixtures from the bottoms of columns, such as *BCD*, are transferred as liquid streams. If thermodynamic efficiency is truly important, one could transfer both a liquid and a vapor stream, and, in certain cases, reboilers and condensers can beneficially be converted to partial reboilers and partial condensers (Agrawal and Fidkowski, 1998 a,b). If needed, it is easy to incorporate such alternate thermodynamic states of the transfer streams within the tabulation of configuration options.

(ii) In both the basic and the thermally coupled configurations, no reboilers or condensers are associated with any of the streams which are recovered from an intermediate location within a distillation column. Streams *BC*, *B*, and *C* in Figure 7c are examples. Sometimes, it makes sense to use either a reboiler or a condenser with such a stream. These situations can arise, for example, if a low-cost heat or refrigeration utility is available at or near the temperatures of these streams. Such situations can also be easily incorporated in the described synthesis method.

(iii) In the method used to identify distinct thermally coupled configurations, a mixture reboiler or condenser from a basic configuration is converted into a simple two-way communication, such as the examples shown in Figure 12. In these examples, the mixture reboiler or condenser is totally eliminated. However, as shown in an earlier study, when a mixture reboiler or condenser is retained, together with the two-way communication, much higher thermodynamic efficiencies can be achieved (Agrawal and Fidkowski, 1999b). Once again, if needed, such modified two-way communications can be easily incorporated in the synthesis method to generate more thermodynamically efficient thermally coupled configurations.

(iv) A general framework was presented in an earlier study whereby the classical two-way communication in a thermally coupled configuration is converted to a one-way liquid-only transfer (Agrawal, 2000a). This conversion is achieved by adding one or more distillation sections, plus a reboiler and/or a condenser with each added section. The resulting equivalent configurations produce some of the component product streams from more than one distillation column. As stated earlier, such configurations can be classified as derived-thermally coupled configurations. The techniques developed for this framework can also be applied to reduce the heat duty of basic distillation column configurations. One consequence of creating such configurations is that it allows the generation of multieffect distillation configurations from thermally coupled configurations. These modifications can be applied to any of the basic and thermally coupled configuration synthesized by the method discussed in this article.

Conclusions

A synthesis procedure for drawing distillation columns to separate n−component mixtures into n product streams each enriched in one of the components is presented. The method synthesizes basic, as well as thermally coupled, configurations.

The basic configurations use $n-1$ distillation columns with each column having a condenser at the top and a reboiler at the bottom. No intermediate reboiler or condenser or two-way communication between the columns is used. A product stream enriched in one of the constituents of the feedstream is produced only once. For ternary mixtures, the three well-known members of basic configurations are the direct split, indirect split, and prefractionator schemes. As expected, the number of basic configurations is found to increase sharply with the increase in the number of components in the feed mixture. The number of basic configurations for four, five, and six component mixtures are found to be 18, 198, and 4,079, respectively. For four-component mixtures, the 18 basic configurations include five well-known configurations with sharp splits between components of adjacent volatility in each distillation column.

The synthesis method for basic configurations is quite easy to use. It is based on the well-known network representation that relates all feasible submixtures that can exist in a distillation column. Some simple observations are described, which are then used to develop a stepwise procedure to create basic configurations. A flowchart of the stepwise procedure is shown in Figure 11. First, each product of intermediate volatility is assigned to be associated with a reboiler, a condenser, or neither. All possible options of these assignments are considered. Implementation of this procedure reduces any n−component option to the equivalent $(n-1)$−component network options. Then, from the prior knowledge of the distillation configurations for the $(n-1)$−component network options, all the distillation configurations for the n−component option are generated. It is asserted that all the basic configurations for a ternary mixture are known. Application of the procedure enables all of the basic four-component configurations to be generated from the three basic ternary configurations. Successive applications will generate 5, 6, . . . n−component configurations from 4, 5,... $(n-1)$−component basic configurations. This allows the creation of all feasible basic configurations for any given multicomponent mixture. If needed, the method can be used for the assignment of all the $n-1$ reboilers and $n-1$ condensers at successive depths within a network to create a final modified network for a specific basic distillation configuration. A shortcut version of the method is also described that quickly yields all feasible basic configurations.

It is found that, for $n>3$, the number of basic configurations declines for options when: (i) a greater number of reboilers and condensers are assigned to product streams of intermediate volatilities; (ii) reboilers are used with intermediate product streams of higher volatilities; or (iii) condensers are used with intermediate product streams of lower volatilities. It is no surprise that the well-known sharp split configurations are contained within those options where all intermediate product streams have associated reboilers and condensers.

Once the basic configurations have been generated, distinct thermally coupled configurations can be readily obtained from the basic ones by systematically replacing mixture reboilers and condensers with two-way communication between distillation columns. While the five thermally coupled schemes using classical two-way communication for ternary mixtures were previously known, the same cannot be said about mixtures containing greater numbers of components. It is found that there are 134 and 5,674 distinct thermally coupled configurations with classical two-way communications for four and five-component mixtures, respectively. If needed, all the thermodynamic equivalent configurations can easily be drawn for any distinct thermally coupled configuration. This will invariably contain more operable configurations that naturally allow for all the vapor streams to flow from a higher pressure to a low pressure. Consequently, no compressors are needed for such transfers. Finally, it is shown that the method is quite versatile and, if needed, it can incorporate various other options regarding the transfer of streams between columns and the use of reboilers and condensers on streams drawn from intermediate locations of distillation columns.

The power of the current method is that it is simple to use, and that it systematically generates not only all of the known basic and thermally coupled distillation configurations, but it also provides many more new configurations. While it is not yet possible to claim that the proposed method is truly exhaustive, it definitely does provide a large number of new distillation configurations. The ultimate advantage of such a method is that it could be incorporated in a search algorithm to systematically find the optimum distillation scheme for a given application. Its use will certainly increase the chance of finding a better solution.

Finally, it is interesting to note that the many new distillation column schemes that are created by the described method also provide an opportunity to draw new membrane cascade and adsorption schemes for multicomponent separations. It was shown in a previous study that n−component membrane cascade schemes can be drawn by a simple analogy with multicomponent distillation schemes for ideal mixtures (Agrawal, 1996b). Recently, the analogy between distillation and simulated moving beds was used to develop candidate simulated moving bed cascades to separate ternary liquid mixtures (Wankat, 2001). The current synthesis method provides an opportunity to draw some new separation schemes in areas other than distillation.

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Appendix: Calculation of Minimum and Maximum Number of Distillation Sections

For an n−component mixture, once reboilers and condensers have been assigned to the intermediate product streams, the minimum and maximum number of possible distillation sections in the resulting basic configurations can be readily calculated. It starts with the observation that in a network representation, every submixture (excluding the product streams) is associated with two distillation sections. Elimination of the recovery and transfer of any of these submixtures between the distillation columns will also reduce the number of distillation sections by two. In other words, absence of any submixture in the final modified network eliminates the associated two distillation sections. In a complete n−component network, such as the ones in Figure 3, there are a total of $n(n-1)$ sections and $n(n-1)/2$ submixtures including feed but excluding n products.

First, consider the calculation of *minimum* number of sections when only a condenser is used with the most volatile component and a reboiler with the least volatile component. In this case, each of the remaining $(n-2)$ condensers and $(n-2)$ reboilers has a submixture (other than the intermediate product streams) associated with it. In order to calculate the minimum number of sections, transfer should be eliminated of all other submixtures between the distillation columns that are not associated with the reboilers and condensers. This implies that in the final network, only these $2(n-2)$ submixtures, feed and the product streams are present. Therefore, accounting for the two sections associated with the feed, the total number of distillation sections for this case are $2[2(n-2)+1] = 4n-6$. For a four-component mixture, configurations in Figures 7a, 7b and 7d with ten sections are such examples.

Now it is easy to calculate the minimum number of sections when reboilers and condensers are associated with the intermediate product streams. For every intermediate product stream that is associated with a reboiler or a condenser, transfer of a submixture stream associated with a reboiler or condenser between the two distillation columns is eliminated. If l is the total number of intermediate product streams associated with reboilers and condensers, then the number of submixtures that are associated either with a reboiler or a condenser and are transferred from one distillation column to another is $2(n-2)-l$. Therefore, the minimum number of distillation sections is $2[(n-2)-l+1] = 4n-6-2l$. For the case when all the intermediate product streams use either a reboiler or a condenser and $l = n-2$, the minimum number of sections $4n-6-2l = 2(n-1)$. For a four component mixture, configurations in Figures 7m−7n are such examples. When only one reboiler or one condenser is used with either component B or C, the minimum number of sections for a four-component mixture is eight. Configurations in Figures 7e−7g are some examples.

In order to calculate the *maximum* number of distillation sections, it is essential to maximize the number of submixtures that are transferred between the distillation columns. In other words, the maximum number of submixtures should be retained in a modified network. When a reboiler or a condenser is assigned to an intermediate product stream, observation 6 provides the basis for the minimum number of the submixtures that must be eliminated from the network (Figures 5, 6 and 8). All the remaining submixtures should be retained to provide the maximum number of distillation sections. For example, consider a case when a condenser is used with C, but no other intermediate product stream uses a reboiler or a condenser. In this case, according to the observation 6, submixtures ABC and BC are eliminated from the network. It leaves $n(n-1)/2-2$ submixtures (including feed, but excluding n products) in the modified network. Therefore, the maximum number of sections equal to $n(n-1)-4$. For a four-component network, the maximum number of sections when a condenser is associated with C is 8. Note that for this four-component case, the minimum and maximum number of sections are the same and there is only one configuration shown in Figure 7e.

When only condensers are associated with intermediate product streams, the maximum number of sections can be readily calculated. Let ν be the volatility rank of a product stream. $\nu = 1$ for the most volatile component A, $\nu = 2$ for the next volatile component B, and so on. Then, use of a condenser with an intermediate product stream of volatility rank ν eliminates $\nu - 1$ submixtures from the network (Figure 5). For all the intermediate product streams with a condenser, all the corresponding values of $\nu - 1$ should be added to calculate the total number of submixtures that are eliminated from the network. Twice the value of this number is then subtracted from $n(n-1)$ to provide the maximum number of sections in the final configuration. As an example, consider a four-component mixture with a condenser at B and C. The corresponding values of $\nu - 1$ are 1 and 2. Therefore, total number of submixtures eliminated is 3. For the maximum number of sections, all other submixtures are retained in the modified network. Therefore, the maximum number of sections are obtained by subtracting 2×3 from 12 ($= n(n-1)$). Note that six is also the minimum number of sections for this case. The only resulting configuration is shown in Figure 7l.

Similarly, when only reboilers are associated with the intermediate product streams, the maximum number of sections possible in a configuration can also be calculated. The use of a reboiler with an intermediate product stream of volatility rank ν eliminates $n - \nu$ submixtures from the network (Figure 8). However, when both reboilers and condensers are assigned to the intermediate product streams, the calculation of submixtures that are eliminated must account for some possible overlaps. Whenever the volatility rank (ν_r) of an intermediate product with a reboiler is higher than the volatility rank (ν_c) of the intermediate product with a condenser, one submixture is common to both the list of eliminated submixtures and the number of eliminated submixtures is $(n - \nu_r) + (\nu_c - 1) - 1$. One should account for all such overlaps to calculate the minimum number of submixtures that must be eliminated from the network to provide the maximum number of feasible sections. As an example, consider a five-component case in Figure 8 where a reboiler is used at B and a condenser at both C and D (option S_{211}). A reboiler B would eliminate 3 ($= 5 - 2$) submixtures. Condensers at C and D by themselves would generally eliminate $2 + 3 = 5$ submixtures. However, for each condenser case, one of the submixtures has already been eliminated by the reboiler at B. Therefore, the total number of eliminated submixtures is $3 + 5 - 2 = 6$. The maximum number of distillation sections in a configuration for this option is $20 - 2 \times 6 = 8$.

Since the distinct thermally coupled configurations are drawn from the basic distillation configurations, the calculation of minimum and maximum number of distillation sections is also applicable to the corresponding distinct thermally coupled configurations (and also to the thermodynamically equivalent configurations).

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