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New Multicomponent Distillation Configurations with Simultaneous Heat and Mass Integration

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In this work, well known Brugma's configurations are shown to be only a subset of a much larger proposed set of simultaneously heat and mass integrated configurations. Furthermore, a systematic classification that allows the exploration of the entire set of simultaneously heat and mass integrated distillation configurations is described. The classification can be used as an underlying principle of any synthesis algorithm and helps identify several novel simultaneously heat and mass integrated distillation configurations for separating a multicomponent feed. A hitherto unknown class of simultaneously heat and mass integrated configurations characterized by strategic side-stream withdrawals is also described. These new configurations provide an array of novel energy efficient options for the nonazeotropic distillation processes. *AIChE J*, 59: 272–282, 2013
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Introduction

Distillation, the method of choice for 90–95% of all separations in the US chemical and petrochemical plants, consumes greater than 40% of the energy used by the chemical and refining industry.[1] Distillation processes can use one or more distillation columns. For instance, to efficiently separate multicomponent mixtures into more than two product streams using distillation, a sequence of distillation columns is usually required. A sequence of distillation columns is also referred to as a distillation configuration or a distillation scheme.

Several attempts have been made to synthesize all possible distillation configurations for a multicomponent separation problem. Early attempts to solve this problem can be traced back to the 1940s,[2,3] and the problem continues to be addressed even in the present. It is important to identify the complete set of alternative arrangements of distillation columns as emphasized by the statement—"If the optimum alternative is not predefined it will not be found."[4]

Figure 1a shows a two-column configuration for separation of a four-component feed mixture. In this configuration and in all other configurations in this article, the volatilities of components decrease in alphabetical order with A being the most volatile component followed by B and so on. Also, reboilers are represented by nonfilled circles, and condensers are represented by filled circles. Further, we refer to streams of intermediate compositions that are transferred between distillation columns as "submixtures." For instance, streams AB and CD are submixtures in the configuration of Figure 1a.

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Additionally, in streams such as AB in Figure 1a, it is not implied that other components such as C and D are completely absent. They may be present but in an acceptably small amount. The configuration shown in Figure 1a is identical to the configuration invented by Brugma,[2] except that the liquid transfer of stream AB is replaced by vapor transfer, because such a vapor transfer would often reduce the total heat duty of the configuration.

Depending on the number of distillation columns in a configuration, a distillation configuration to separate an n-component feed into n product streams has been classified as a "plus-column," a "regular-column" or a "subcolumn" configuration.[5] Distillation configurations with more than $n - 1$ distillation columns are plus-column; with exactly $n - 1$ columns are regular-column; and with less than $n - 1$ columns are subcolumn configurations. The Brugma configuration[2] of Figure 1a is a subcolumn configuration, as it uses two distillation columns for a four-component separation.

Sometimes thermal coupling links are introduced between distillation columns in a configuration to reduce the total heat duty requirement of distillation.[6–8] Thermal coupling links are two-way liquid–vapor communications between distillation columns of a configuration. Reboilers or condensers that involve one-way transfers of submixtures in a configuration can be replaced with thermal coupling links. Consequently, distillation configurations can be classified as partially or completely thermally coupled configurations depending on the number of reboilers or condensers in these configurations that are replaced by thermal coupling links.[9] In configurations with complete thermal coupling, all of the replaceable reboilers and condensers have thermal coupling links. In configurations with partial thermal coupling, at least one of the replaceable reboilers or condensers does not have a thermal coupling link. The configuration shown in Figure 1b

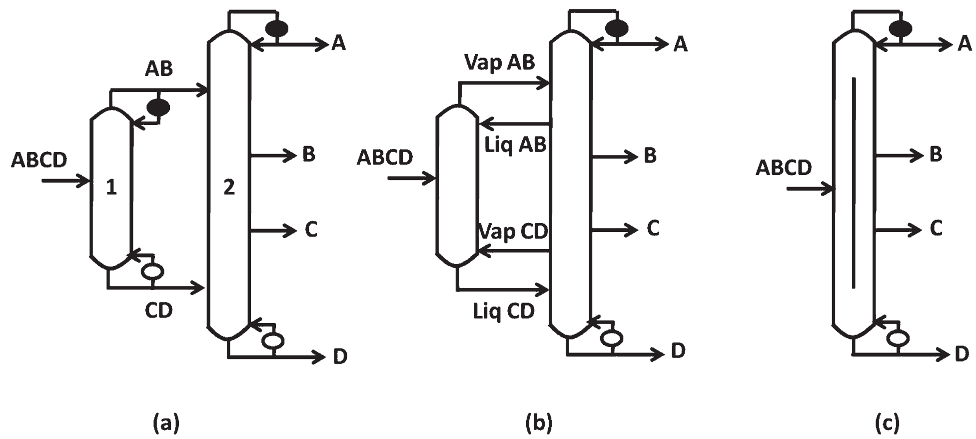

Figure 1. Some known simultaneously heat and mass integrated configurations.

(a) Brugma configuration,[2] (b) Cahn and Di Miceli configuration,[10] and (c) Kaibel configuration.[11]

is a completely thermally coupled analog of the Brugma configuration[2] of Figure 1a and was described by Cahn and Di Miceli.[10]

It is known that two or more thermally coupled columns can be essentially combined into a single shell using a dividing wall column.[6,11–14] For instance, the distillation columns in Figure 1b can be combined into a single shell as shown in Figure 1c. The well-known Kaibel column configuration[11] of Figure 1c is thus a dividing wall column version of the Cahn and Di Miceli configuration.[10]

For nonazeotropic mixtures, basic distillation configurations[9] are regular-column configurations with each column having one reboiler and one condenser. Basic configurations have the ability to produce all the products of any prespecified purity. The subcolumn Brugma configuration[2] (Figure 1a) is obtained from a basic regular-column distillation configuration by simultaneous heat and mass integration of distillation columns as illustrated in Figure 2. In the basic configuration of Figure 2a, the bottom product of the second distillation column is stream B, whereas the top product of the third distillation column is stream C. As the bottom product of the second distillation column is more volatile than the top product of the third distillation column, the two columns can be heat and mass integrated without disturbing the composition profiles in the individual distillation columns by introducing an additional column section with sufficient separation stages. The additional section eliminates reboiler associated with stream B and condenser associated with stream C. It also connects the two distillation columns "2" and "3" of the basic configuration in Figure 2a to provide one column in Figure 2b, which does the same overall separation. The task of the additional heat and mass integrated section is to do mass exchange between the ascending C-rich vapor from the bottom section of the column and the descending B-rich liquid from the top section of the column to provide B-rich vapor stream for the top section and C-rich liquid stream for the bottom column section. The subcolumn configuration retains the ability of the basic regular-column configuration from which it is derived to make arbitrarily high purity products provided that there are sufficient separation stages in the additional column section.

Simultaneous heat and mass integration of distillation columns not only reduces the number of distillation columns and reboiler/condenser heat exchangers in a configuration but also decreases the total heat duty requirement of the configuration. The total vapor duty requirement of a configuration is the sum of the vapor flows generated at the reboilers of a configuration and is proportional to the heat duty requirement of a configuration.[15] Through simultaneous heat and mass integration, the sum of the heat duty requirements of the two individual distillation columns is replaced by the greater of the two heat duties. The distillation column with the lower heat duty requirement operates for "free," because its required vapor flow is borrowed from the other

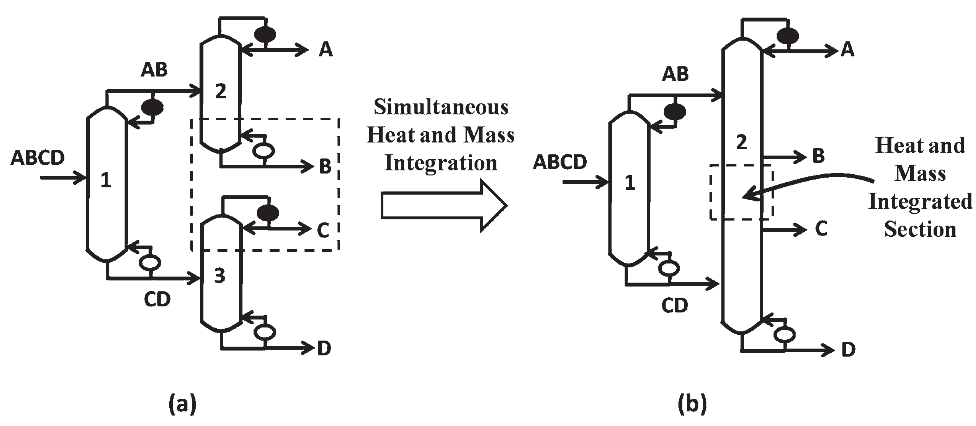

Figure 2. Use of a simultaneous heat and mass integration section to convert a regular-column configuration into a subcolumn Brugma configuration[2] of Figure 1a.

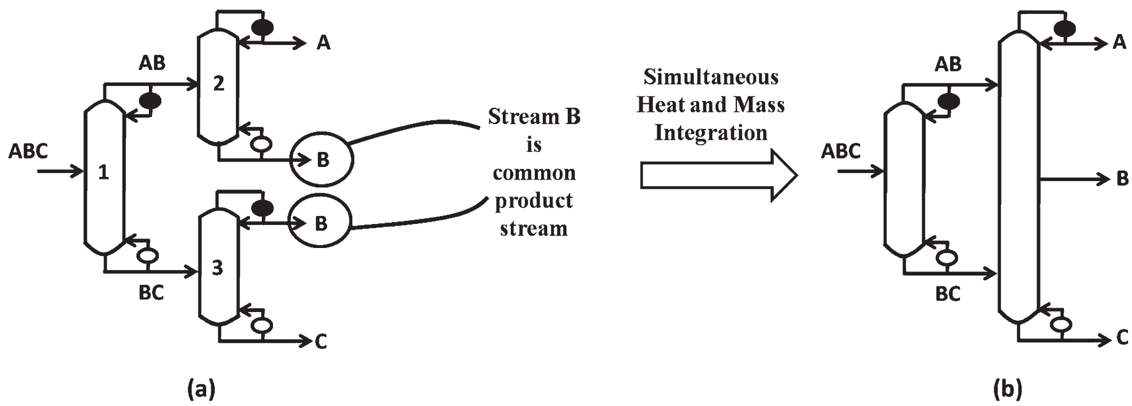

Figure 3. Illustration of simultaneous heat and mass integration of distillation columns producing the same pure products.

distillation column with which it is heat and mass integrated. To illustrate, for a given separation, let V_1, V_2, and V_3 be the vapor flow requirements of distillation columns "1," "2," and "3," respectively, of the configuration shown in Figure 2a. The total vapor flow requirement of the configuration of Figure 2a is thus given by

$$V_{[\text{before heat and mass integration}]} = V_1 + V_2 + V_3 \tag{1}$$

Due to simultaneous heat and mass integration of the second and third distillation columns of the configuration shown in Figure 2a, the total minimum vapor flow requirement of the configuration of Figure 2b is

$$V_{[\text{after heat and mass integration}]} = V_1 + \max(V_2, V_3) \tag{2}$$

It is evident from Eqs. 1 and 2 that

$$V_{[\text{after heat and mass integration}]} < V_{[\text{before heat and mass integration}]} \tag{3}$$

Another example of a simultaneously heat and mass integrated configuration is illustrated in Figure 3. Petlyuk et al.[7] demonstrated that distillation columns producing final product streams of same composition can be simultaneously heat and mass integrated. Figure 3a shows a three-column distillation configuration for separating a three-component feed. In the configuration of Figure 3a, final product stream B is produced as the bottom product of the second distillation column and as the top product of distillation column 3. As a stream with same composition is produced from a reboiler as well as a condenser, Petlyuk et al.[7] eliminated the associated exchangers and combined column 2 with column 3 of the configuration in Figure 3a into a single shell. Consequently, they obtained the basic configuration with simultaneous heat and mass integration shown in Figure 3b.

Similar to simultaneous heat and mass integration between distillation columns producing final product stream of same composition (Figure 3), distillation columns producing submixtures of same components have also been heat and mass integrated.[16–19] An example of such a configuration is shown in Figure 4. The basic configuration of Figure 4b is obtained by simultaneous heat and mass integration of the second and third distillation columns in the configuration of Figure 4a. The reboiler and condenser associated with the common submixture BC in the configuration of Figure 4a are eliminated, and stream BC is produced as a side-draw stream from the heat and mass integrated column. One observes that the simultaneous heat and mass integration of columns producing streams of the same components, either final product streams (Figure 3) or submixtures (Figure 4), does not require an additional intermediate section.

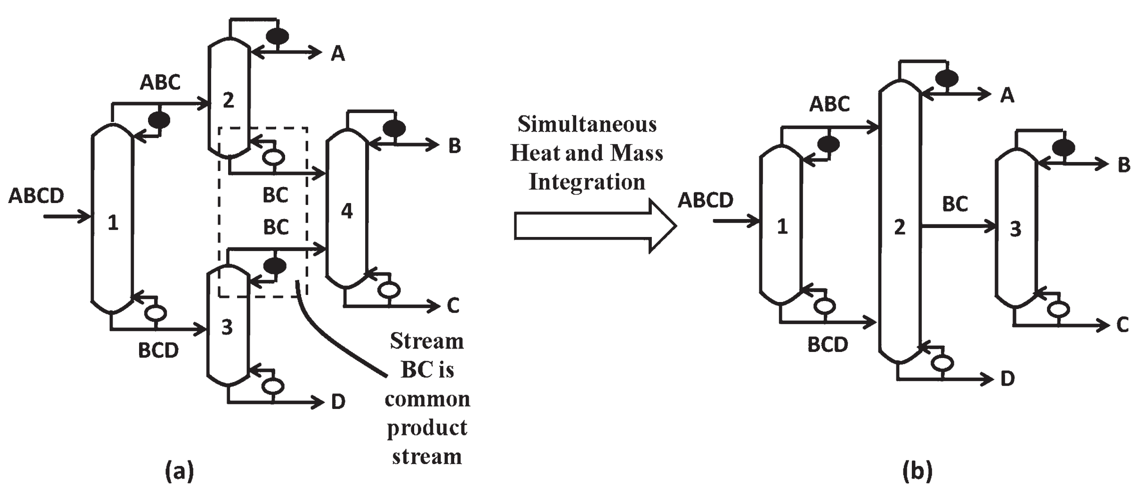

Figure 4. (a) A four-column configuration for separating a four-component mixture and (b) a basic configuration derived by simultaneous heat and mass integration of second and third distillation columns in (a).

The early work on simultaneous heat and mass integration involved combining distillation columns producing final product streams of same or different components.[2,7] In parallel, several synthesis algorithms that captured simultaneous heat and mass integration between columns producing submixtures of same components were developed by researchers.[5,9,16–19] Rong et al.[20–23] considered combining distillation columns producing submixtures of different components, but they considered only heat integration without any mass integration between these distillation columns. Fidkowski[24] proposed a rule to consider all possibilities for combining columns producing streams of the same components.

In this work, we have developed a systematic classification to identify all possible combination of distillation columns that can be simultaneously heat and mass integrated for separation of nonazeotropic mixtures. We find that there are several previously unexplored possibilities of simultaneous heat and mass integration between distillation columns, and we demonstrate their energy-saving potential with the help of a case study. Some of the unexplored configurations lead to an entirely new class of hitherto unknown configurations with strategic side-stream withdrawals. These configurations have potential to provide further benefits in lowering the heat duty requirement.

Heat and Mass Integration Links and Their Classification

For the purpose of this article, we define a heat and mass integration link as a two-way communication between distillation columns that involves the elimination of a reboiler associated with a first distillation column and a condenser associated with a second distillation column followed by combining the columns into a single shell. A heat and mass integration link differs from a thermal coupling link as (a) it requires simultaneous elimination of both a reboiler and a condenser from two different distillation columns, (b) it involves combining the two columns into a single column shell, and (c) it does not necessarily involve reboilers and condensers associated with only submixtures. For example, the Brugma configuration[2] of Figure 2b is obtained by introducing a heat and mass integration link between the second and third columns producing final product streams in the configuration of Figure 2a. On the other hand, a thermal coupling link can be introduced in the Brugma configuration[2] by eliminating the condenser associated with submixture AB. Separately, a second thermal coupling link can be introduced by eliminating reboiler associated with submixture CD. This consequently provides the Cahn and Di Miceli configuration[10] shown in Figure 1b.

We refer to a distillation column obtained by simultaneous heat and mass integration of the two distillation columns as a simultaneously heat and mass integrated column. Also, the distillation configuration with a simultaneously heat and mass integrated column is referred to as a simultaneously heat and mass integrated configuration. Thus, the Brugma configuration[2] of Figure 2b is a simultaneously heat and mass integrated configuration with the second distillation column being a simultaneously heat and mass integrated column. By our definition, the configurations shown in Figures 3b and 4b are also simultaneously heat and mass integrated configurations.

We classify simultaneous heat and mass integration between columns into three categories based on the types of streams associated with the distillation columns that are heat and mass integrated. A simultaneous heat and mass integration link can be introduced by eliminating a reboiler and a condenser associated with (a) two final product streams, or (b) two submixtures, or (c) a submixture and a final product stream.

(a) Combining two distillation columns with each producing a final product stream

We can obtain simultaneously heat and mass integrated columns by introducing heat and mass integration links between columns producing final product streams of either the same or different compositions (Figures 3 and 2, respectively). When product streams of different compositions are involved, the component being vaporized in the eliminated reboiler is lighter than the component being condensed in the eliminated condenser. It is worth noting that Christiansen et al[25] pointed out operational difficulties in the Brugma configuration[2] and its thermally coupled analogs[10,11] shown in Figure 1. They observed that in industrial practice, it may be difficult to operate the intermediate heat and mass integrated section between the withdrawal locations of final products B and C. This may consequently prevent the side-stream products from being of extremely high purities. However, the Kaibel configuration[11] (Figure 1c) for separation of a mixture into four pure product streams is currently being successfully operated in the chemical industry.[26–29] Also, several researchers[27,30] are involved with improving the design and control of the four-product Kaibel column.

(b) Combining two distillation columns with each producing a submixture stream

Similar to simultaneous heat and mass integration of distillation columns producing final product streams, we can introduce heat and mass integration links between columns producing submixtures. An example of a configuration with simultaneous heat and mass integration between columns producing submixtures of same components has been presented in Figure 4.

A previously unexplored option of simultaneous heat and mass integration is between distillation columns producing submixtures that contain some non-overlapping components. Such a simultaneous heat and mass integration is illustrated in Figure 5. Consider a basic distillation configuration for separating a five-component feed into five product streams shown in Figure 5a. In this configuration, distillation column 2 produces submixture BC as the bottom product and column 3 produces submixture CD as the top product. We introduce a heat and mass integration link in the configuration of Figure 5a by eliminating the reboiler and condenser associated with the lighter BC and the heavier CD streams, respectively, and combining distillation columns 2 and 3 after introducing sufficient separation stages between the two distillation columns. This results in the simultaneously heat and mass integrated configuration with the associated additional intermediate section in column 2 (Figure 5b). Sufficient separation stages are required in the additional intermediate section to ensure a smooth transition in the composition profile between the two ends of this section. The additional section in this figure as well as subsequent figures is shown by a dotted box.

It is worth noting that the configuration of Figure 5b demonstrates heat and mass integration between columns producing submixtures BC and CD that have only one overlapping component C. Alternatively, heat and mass

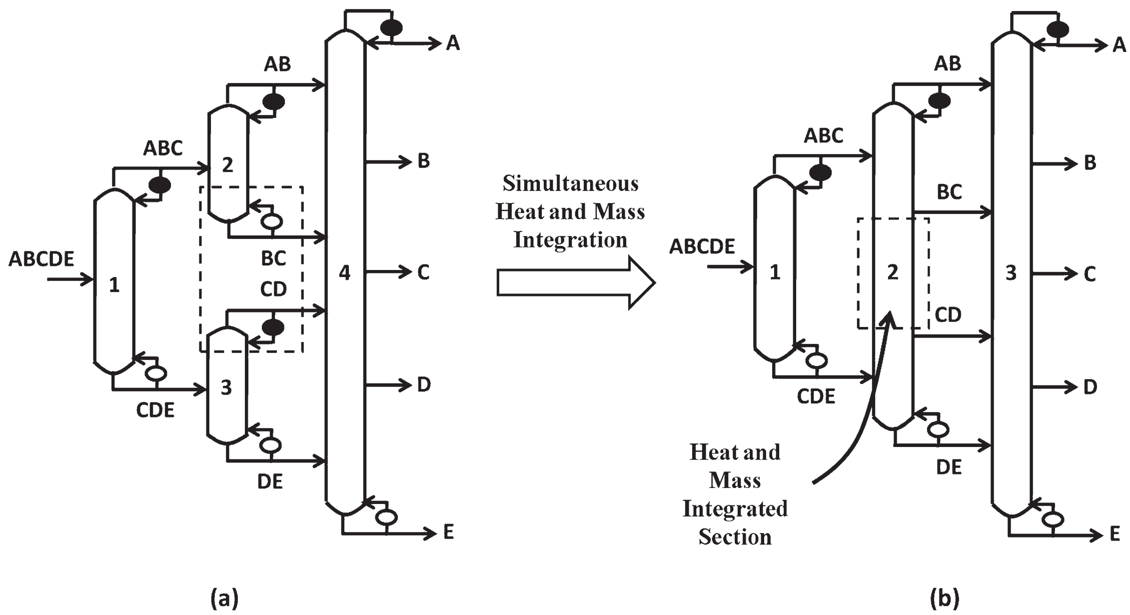

Figure 5. (a) A basic distillation configuration for five-component separation and (b) a new simultaneously heat and mass integrated configuration.

integration links can be introduced between columns producing submixtures with more than one overlapping components as well as with no overlapping components. Examples of such configurations are shown in Figure 6. In the configuration of Figure 6a, vapor BCD and liquid CDE submixture streams, having common components C and D, are produced from the heat and mass integrated column. On the other hand, the configuration of Figure 6b produces submixtures vapor BC and liquid DE that have no overlapping components from the heat and mass integrated column.

In summary, this category of heat and mass integration links can be further categorized into three subcategories as:

(b1) Both submixtures have same components.

(b2) Not all but only some of the components are common between the two submixtures.

(b3) None of the components are common between the two submixtures. In this case, all the components in the submixture from the reboiler are more volatile than any component in the submixture from the condenser.

To our knowledge, among the three subcategories, only simultaneously heat and mass integrated configurations corresponding to subcategory (b1) have been previously known in the literature.

(c) Combining two distillation columns with one producing a submixture stream and the other producing a final product stream

Figure 7 shows examples of simultaneously heat and mass integrated configurations obtained by introducing a heat and mass integration link between a distillation column

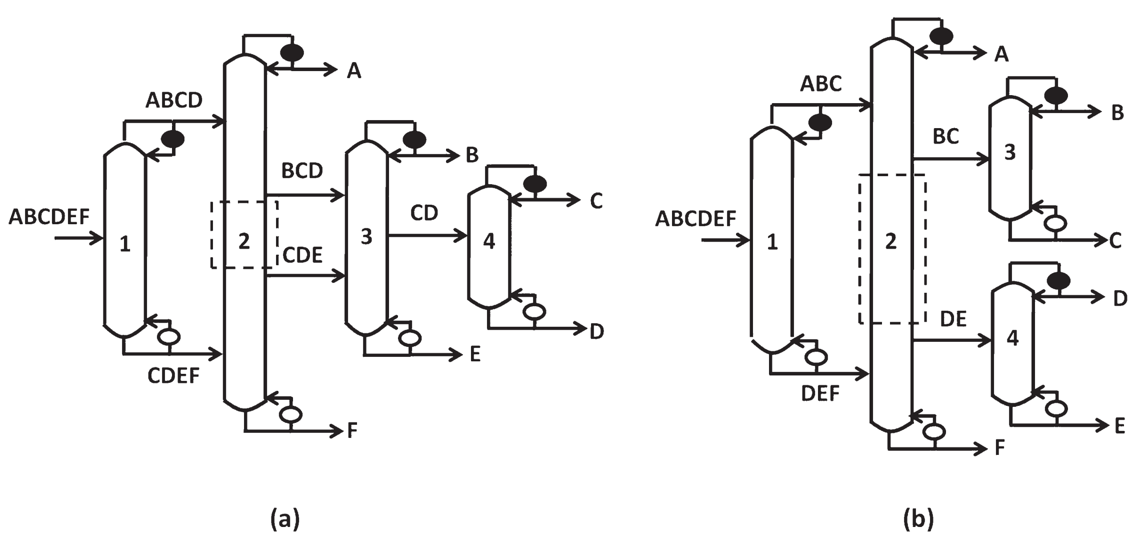

Figure 6. Examples of simultaneously heat and mass integrated configurations obtained by combining distillation columns producing submixtures that contain non-overlapping components.

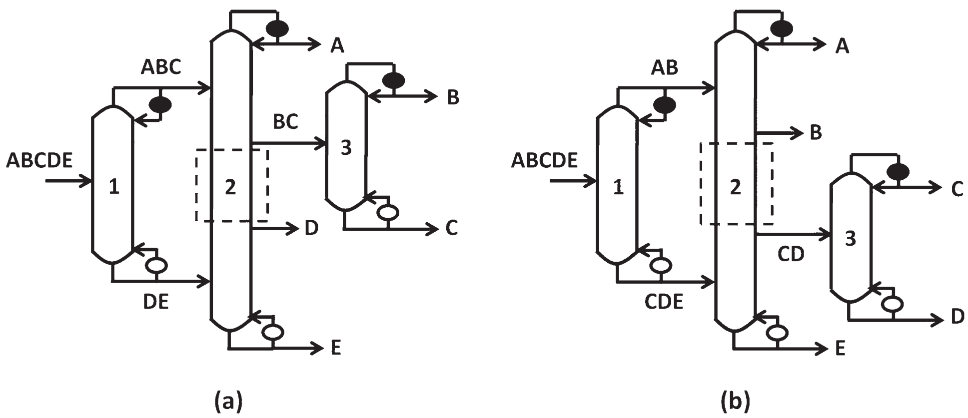

Figure 7. Examples of simultaneously heat and mass integrated configurations obtained by combining columns producing a submixture and a final product stream.

producing a submixture and a distillation column producing a final product stream. By definition, a submixture and a final product stream will always have different compositions. This consequently implies that the simultaneously heat and mass integrated columns belonging to this category will always involve an additional intermediate column section in the heat and mass integrated column. To our knowledge, such simultaneously heat and mass integrated configurations have also not been previously explored in the literature.

Such a formal classification of heat and mass integration links into three distinct categories (a–c) facilitates systematic identification of the complete set of all possible simultaneously heat and mass integrated configurations for a multicomponent separation. This classification can be included in any available synthesis framework to generate additional feasible distillation configurations for separating a multicomponent mixture.

Although the examples (Figures 2–7) have only involved one of the three categories of heat and mass integration links, we can have configurations with multiple heat and mass integration links of any type as illustrated in Figure 8. The simultaneously heat and mass integrated configuration of Figure 8b is obtained from the basic configuration shown in Figure 8a by introducing heat and mass integration links between columns 2 and 3 that produce two submixtures as well as between columns producing two final products, that is, columns "4" and "5." The configuration in Figure 8b could also be derived from the one in Figure 6b.

Furthermore, simultaneously heat and mass integrated configurations can be obtained not only from basic configurations but also from subcolumn and plus-column configurations. The simultaneously heat and mass integrated configurations obtained by combining columns producing streams containing same components have already been accounted for in the search space of basic configurations[9,18,19,31] and subcolumn configurations.[5] However, configurations with simultaneous heat and mass integration between distillation columns producing streams containing at least some different components, including some of the new configurations described in this article (Figures 5–8), have not been systematically synthesized in the literature.

Shah and Agrawal[19] introduced a six-step matrix-based method to synthesize the complete search space of basic regular-column configurations for separating a nonazeotropic multicomponent feed mixture. They built on the observations proposed by Agrawal[9,17] and developed the matrix method

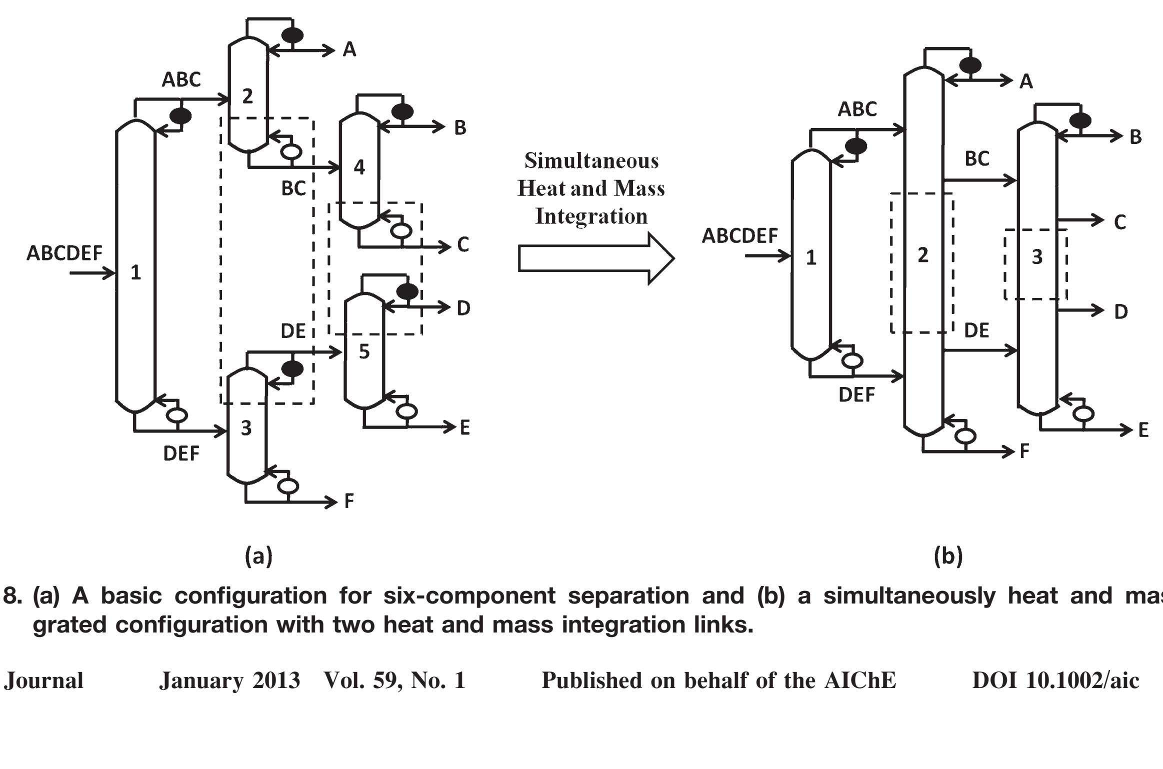

Figure 8. (a) A basic configuration for six-component separation and (b) a simultaneously heat and mass integrated configuration with two heat and mass integration links.

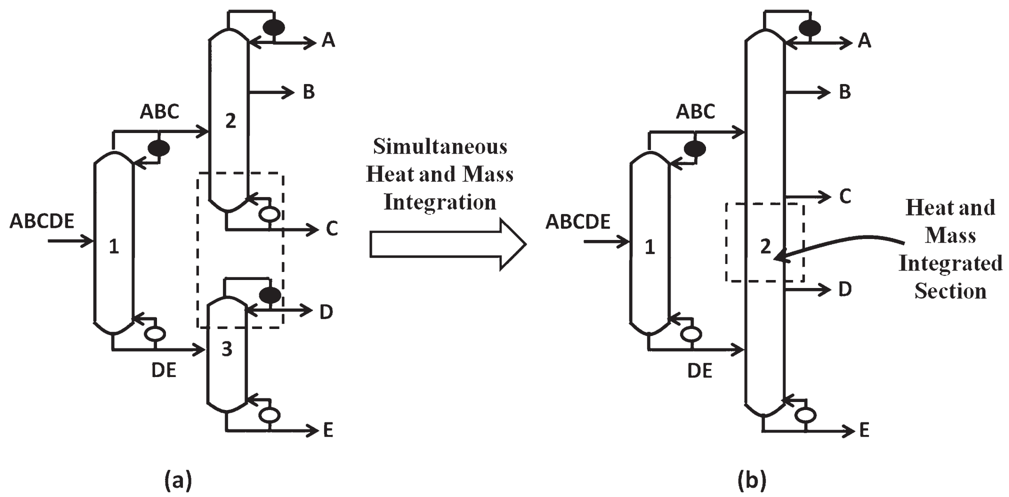

Figure 9. (a) Subcolumn configuration for five-component separation and (b) simultaneously heat and mass integrated configuration obtained from subcolumn configuration in (a).

in which distillation configurations are generated by exploring all possible instances of the presence or absence of submixtures. Shenvi et al.[5] added two new steps to the matrix-based approach of Shah and Agrawal[19] to generate the complete set of subcolumn configurations by introducing the concept of product zones. Using the formal classification presented in this article, we have extended the matrix method to generate the complete search space of simultaneously heat and mass integrated configurations that can be derived from plus-column, regular-column, and subcolumn configurations. This synthesis approach computationally explores all possible combinations of heat and mass integration links. Details of this extended matrix method will be provided in a follow-up article.

It is worth mentioning that for simultaneous heat and mass integration of distillation columns producing streams containing non-overlapping components, we require that at least one of the two conditions must be satisfied: (1) the stream from the condenser contains at least one component that is less volatile than any component present in the reboiler stream and (2) the reboiler stream contains at least one component that is more volatile than any of the components present in the condenser stream. This also implies that the stream associated with the reboiler should have a bubble point temperature that is lower than the dew point temperature of the stream associated with the condenser (after accounting for an appropriate pressure drop; Figures 2 and 5–8). This would ensure that the more volatile stream would be produced at a location above that of the less volatile stream in the heat and mass integrated column.

Simultaneously heat and mass integrated configurations obtained from basic configurations retain the ability of the basic configurations to produce products of any prespecified purity (Figures 2 and 5–8). For this purpose, sufficient separation stages are required in the additional heat and mass integrated sections. However, some subcolumn configurations do not have the ability to produce all the products of arbitrarily high purity. For instance, in the configuration of Figure 9a, the second column produces product stream B as a side-stream above the location of the feed ABC. Consequently, this side-draw stream B will be contaminated in the lighter component A. We can maximize the purity of stream B by increasing the reflux in the second column but producing stream B of very high purity will require significantly large energy. The simultaneously heat and mass integrated configuration derived from the configuration of Figure 9a is shown in Figure 9b. Similar to the subcolumn configuration of Figure 9a, the simultaneously heat and mass integrated configuration will also not be able to make product stream B of arbitrarily high purity (without a large energy penalty).

Case Study

To demonstrate the energy-saving potential of simultaneous heat and mass integration of distillation columns, we use ASPEN Plus® to simulate the configurations in Figure 5. Our objective is to compare the total reboiler duty of the basic configuration of Figure 5a with the new simultaneously heat and mass integrated configuration of Figure 5b that is obtained by combining columns producing submixtures of different compositions.

The first distillation column in the two configurations of Figure 5 performs the same separation task of separating feed ABCDE into streams ABC and CDE. However, for a given separation, when the total heat duty of each configuration is minimized, the reboiler duty of the first column could be different between the two configurations. At optimal performance, the composition of the streams ABC and CDE necessarily may not match between the two configurations. To simplify our simulation and to illustrate the energy-saving potential of the simultaneous heat and mass integration of columns in Figure 5b, we assume streams ABC and CDE to have the same compositions in both the configurations. In our simulation, this led to comparing the reboiler duties of distillation columns 2, 3, and 4 in the configuration of Figure 5a with the second and third distillation columns of the configuration shown in Figure 5b.

We consider the separation of a five-component mixture comprising of *n*-pentane (A), 2,2-dimethylpentane (B), 2-methlyhexane (C), *n*-heptane (D), and *n*-nonane (E). The five final products are desired to have at least 98% purity (in mole percent). The second, third, and fourth distillation columns in the configuration of Figure 5a and second and third distillation columns of the configuration shown in Figure 5b are simulated and optimized using the

Table 1. Stream Data Used for the Simulations of the Configurations in Figures 5 and 11

	Feed Stream	
	ABC	CDE
Component flow (kmol/h)		
A	5	0
B	10	0
C	35	35
D	0	10
E	0	5
Total flow (kmol/h)	50	50
Vapor fraction	1	0

stage-by-stage distillation model RADFRAC in Aspen Plus®. The NRTL model is used to calculate the activity coefficients in the simulations.

The component flows of the feed streams ABC and CDE to the second and third distillation columns of Figure 5a and to the second distillation column of Figure 5b are provided in Table 1. In this table, stream ABC is saturated vapor, and stream CDE is saturated liquid. The pressure of each distillation column in the simulations is fixed to 3 atm. Also, all distillation columns are simulated with 200 separation stages. Such a large number of stages enables each column section to have more than enough stages ensuring that the simulation results are relatively insensitive to the exact tray location of the feeds and the side-draw products. All the final product streams are produced as liquid. The submixtures associated with reboilers are produced as liquids, and the submixtures associated with condensers are produced as vapors. Although not essential, in the simulation of Figure 5b, submixture BC is produced as a liquid stream and submixture CD is produced as vapor. The flow rates of the submixtures and reflux ratios of the distillation columns are considered as variables in the ASPEN Plus® optimization algorithm.

Table 2 provides the simulation details and results obtained for the configurations shown in Figure 5. We find that the total reboiler duty of the second and third columns in the simultaneously heat and mass integrated configuration of Figure 5b is lower by around 19% than the total reboiler duty of columns 2, 3, and 4 of the configuration of Figure 5a. This case study clearly illustrates the energy-saving potential of the new

Table 2. Examples of Energy Savings from the Novel Distillation Configurations

	Figure		
	5a	5b	11
Stage locations from the top	Column 2 ABC in – 100 Column 3 CDE in –100 Column 4 AB in – 10 BC in – 60 CD in – 140 DE in – 190 B out – 20 C out – 100 D out – 180	Column 2 ABC in – 40 CDE in –160 BC out – 80 CD out – 120 Column 3 AB in – 10 BC in – 60 CD in–140 DE m–190 B out – 20 C out – 100 D out – 180	Column 2 ABC in – 40 CDE in –160 BC out – 80 C out –85 CD out – 120 Column 3 AB in –10 BC in – 60 CD in – 140 DE in – 190 B out – 20 C out – 100 D out – 180
Total reboiler duty (kW)	2669	2170	1965

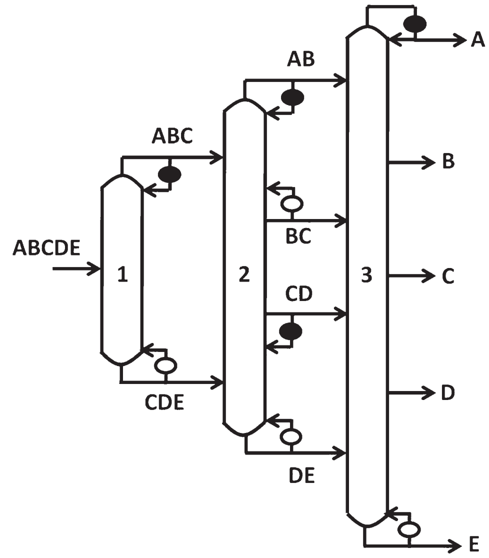

Figure 10. Heat and mass integrated configuration with intermediate reboiler and intermediate condenser.

simultaneously heat and mass integrated configurations for multicomponent separation. Therefore, all such configurations must be included in a search space of distillation configurations to separate any multicomponent mixture.

Further, the heat and mass integrated configuration of Figure 5b uses one less distillation column as well as one less reboiler and condenser as compared to the configuration of Figure 5a. However, simultaneous heat and mass integration of distillation columns requires additional cost considerations with regard to the possible need of additional separation stages to attain desired purities of the side-streams. For instance, sufficient stages need to be provided in the heat and mass integrated section of the configuration (Figure 5b) between product withdrawal locations of streams BC and CD to ensure that the amounts of components D and B in streams BC and CD, respectively, are lower than their acceptable limits.

Another aspect to consider in the simultaneously heat and mass integrated configurations of Figure 5b is the possible second law penalty because of increased heat demand at higher temperature or increased cooling demand at lower temperatures. The total vapor flow requirement of the configuration of Figure 5b is less than that of the configuration in Figure 5a, but now more vapor may need to be generated at the higher-temperature reboiler DE as compared to providing some of the heat at the lower temperature reboiler BC in the configuration of Figure 5a. Alternatively, more vapor may need to be condensed at the lower temperature condenser AB in configuration of Figure 5b. Thus, although simultaneous heat and mass integration can provide a potential first-law energy benefit in terms of lower total heat demand, it may incur a temperature-level energy penalty. Intermediate reboilers/condensers can be introduced at appropriate locations in the simultaneously heat and mass integrated distillation column to avoid the second law penalty if required.[13,32] Figure 10 shows configuration with intermediate reboiler and intermediate condenser introduced in the second distillation column of the heat and mass integrated configuration in Figure 5b. In this article, we have not considered the capital cost or configurations having reboilers and condensers at

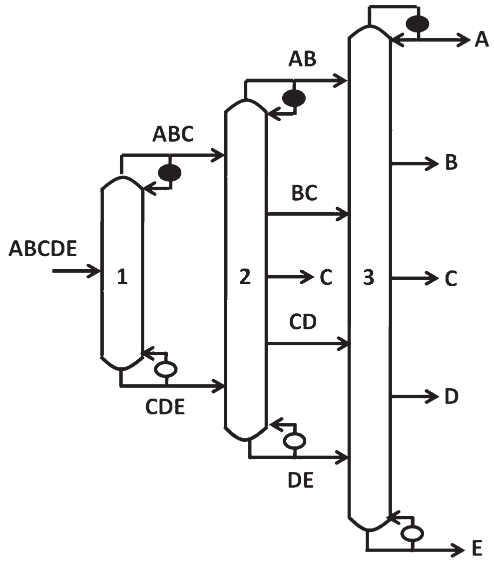

Figure 11. Novel simultaneously heat and mass integrated configuration with an additional side-product stream withdrawal for five-component separation.

intermediate column locations. Such additional considerations can also be included when appropriate.

Strategic Side-Stream Withdrawal—Novel Heat and Mass Integrated Configurations

Interestingly, the new simultaneously heat and mass integrated configurations that we have obtained by combining distillation columns producing submixtures of different compositions (for instance, Figure 5) offer a unique opportunity to withdraw additional side-stream products. Consider the simultaneously heat and mass integrated configuration shown in Figure 5b. This configuration utilizes an additional section between the withdrawal locations of streams BC and CD in the second distillation column with component C being common between the two streams. We hypothesize that if sufficient stages are provided in this additional section, component C will almost completely separate out from streams BC and CD in the intermediate stages of this section. In such a case, the composition profile of the overlapping component C will go through a maximum in the heat and mass integrated column, and at the corresponding separation stage, we will have almost pure component C in the column. As the separation objective is to eventually obtain pure product stream C, it will be more efficient to withdraw some permissible amount of product C from the additional section between the withdrawal locations of product streams BC and CD where a peak in the composition of C would be exhibited. This results in a hitherto unknown distillation configuration as shown in Figure 11. Note that stream C is now produced at two locations, from the second and the third distillation columns.

To illustrate the efficacy of the novel configuration with heat and mass integration and an additional side-product stream shown in Figure 11, we compare the total reboiler duty of this configuration with the configurations in Figure 5. For this purpose, we simulated the process of Figure 11 for the same process specifications as for Figure 5, and the results are shown in Table 2. Figure 12 shows the composition profile for component C in the second distillation

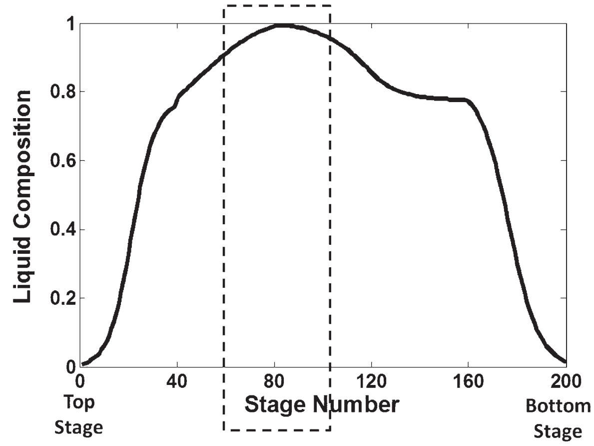

Figure 12. Component C composition profile in the second column of the simultaneously heat and mass integrated configuration of Figure 5b.

column of the configuration shown in Figure 5b. The box in Figure 12 corresponds to the separation stages in the section between the withdrawal locations of streams BC and CD. The composition profile indicates that pure C is present in the simultaneously heat and mass integrated column. It is, therefore, no surprise that by merely withdrawing an extra product stream from the configuration of Figure 5b, we can further reduce the heat duty requirement using the configuration of Figure 11 (Table 2). The second and third distillation columns in the configuration of Figure 11 have around 10% lower total reboiler duty requirement than the corresponding distillation columns in the configuration shown in Figure 5b and also provide around 26% savings as compared to the columns 2–4 in the configuration of Figure 5a. Of course, if all the three columns were simultaneously optimized for lower heat duty, we expect the benefit of the Figure 11 configuration to be greater than what the simulations have illustrated here. Thus, these new simultaneously heat and mass integrated configurations with additional side-product streams have significant potential for saving in the operating costs.

We can extend the concept of strategic side-stream withdrawals to other heat and mass integrated configurations that are obtained by combining columns producing submixtures of different compositions. The configuration of Figure 6a is obtained by simultaneously heat and mass integrating distillation columns producing streams BCD and CDE. Submixtures

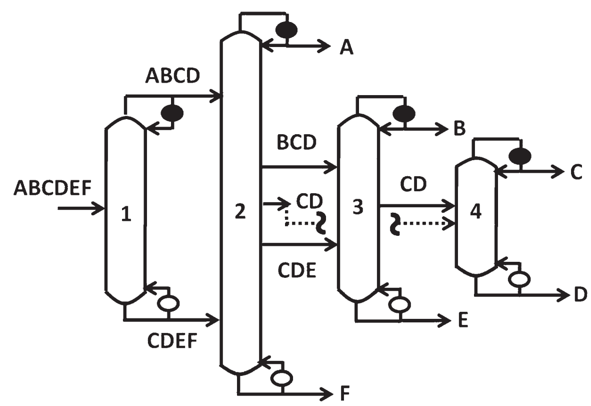

Figure 13. A novel simultaneously heat and mass integrated configuration with an additional side-stream for a six-component separation.

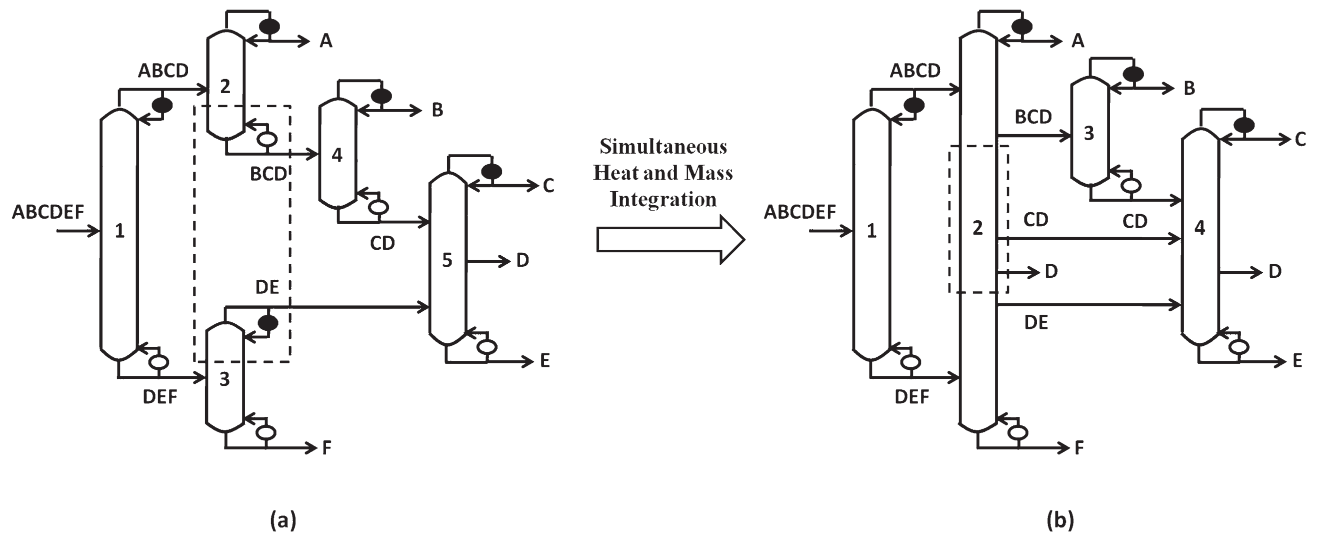

Figure 14. (a) A regular-column six-component configuration and (b) a corresponding simultaneously heat and mass integrated configuration with additional side-submixture and product streams.

BCD and CDE have two common components, namely, C and D. If we provide sufficient stages in the section of the second column in the configuration of Figure 6a between withdrawal locations of BCD and CDE, then there will be a location where concentrations of components B and E will be negligibly low and the liquid and vapor streams will be primarily composed of C and D. Consequently, we can produce stream CD at that corresponding stage in the column. This yields the novel configuration shown in Figure 13. This configuration has an additional submixture stream CD produced from the heat and mass integrated distillation column 2, which is subsequently fed to the fourth distillation column for further distillation into product streams C and D. It must be noted that the relative feed locations of the two CD streams to the fourth distillation column will be decided by appropriate flow sheet optimization.

Of course, it is also possible to have configurations where we have resulting additional submixture as well as product streams due to the simultaneous heat and mass integration between the columns. Such an example is shown in Figure 14. The simultaneous heat and mass integration between columns 2 and 3 of Figure 14a results in additional submixture side-stream CD and product side-stream D from column 2 of Figure 14b.

It should be pointed out that from a simultaneous heat and mass integrated column configuration such as the one in Figure 8b, it is possible to draw more than one product stream. In column 2, we have an integrated section where two binary streams BC and DE enter from the top and the bottom, respectively, and there is no overlapping components between them. In such a case, depending on the number of stages in this section, we have multiple possibilities. If the number of stages is not large, one could withdraw a side-stream CD mainly composed of C and D only. This stream could be fed at an appropriate location of the third column. The resulting configuration is shown in Figure 15a. In a rare situation, where a mixture stream CD may be needed as a product stream or an input to a downstream unit operation, the withdrawn stream CD could be used for that purpose. On the other hand, if large enough trays are used in this section, one could coproduce both a pure C and a pure D product streams from this section as shown in the configuration of Figure 15b.

Our synthesis method (to be described in a subsequent article) also includes steps to systematically generate these novel configurations with strategic side-stream withdrawals, for inclusion in the search space of configurations for multicomponent distillation.

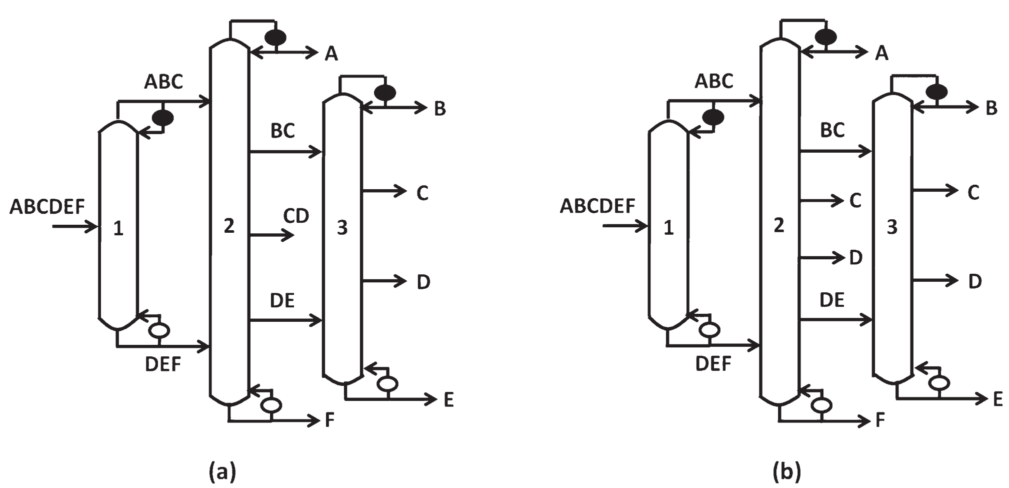

Figure 15. Examples of configurations with additional side-streams obtained from the simultaneously heat and mass integrated configuration in Figure 8b.

Conclusions

While generating distillation configurations, it is customary to combine two columns into one column when the bottom of one column produces a submixture stream containing the same components as the top of another column. Here, we suggest that certain other configurations such as the one from Brugma[2] are the result of simultaneous heat and mass integration between the two columns, whereby the bottom of one column producing a light product stream is integrated with the top of another column producing a heavier product stream. Such an integration between the two columns is achieved by replacing the associated reboiler and condenser with an additional section in the resulting column.

In this work, we have provided a systematic classification framework for all possible simultaneous heat and mass integrated links that enable identification of potential columns that can be integrated as such. As a result of our definition and classification, we find that there are several options of simultaneous heat and mass integration between distillation columns that have not been considered previously. Through our proposed methodology, we have identified new heat and mass integrated configurations that can be obtained by combining distillation columns producing submixtures and final product streams of different compositions. This new class of configurations holds the promise to be more energy-efficient while using lower number of columns than regular-column configurations.

Additionally, the new heat and mass integrated configurations provide further opportunities to strategically withdraw additional final product or submixture streams as side-streams. This results in a special class of hitherto unknown configurations with simultaneous heat and mass integration and additional side-stream withdrawal. Such additional side-streams further decrease the heat duty of a configuration containing the simultaneously heat and mass integrated column.

Through a case study for five-component mixture separation, we have demonstrated the potential of the new heat and mass integrated configurations as well as configurations with additional side-stream products to provide substantial energy benefits. This case study demonstrates the need to include this new class of configurations in a search space of configurations for separating a given multicomponent mixture.

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