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Synthesis and Optimal Design of Thermodynamically Equivalent Thermally Coupled Distillation Systems†

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A thermodynamically equivalent structure (TES) is the distinct feature of a thermally coupled configuration. This paper presents the synthesis and optimal design of thermodynamically equivalent thermally coupled systems for multicomponent distillations. First, the original thermally coupled configurations (OTCs) for traditional distillation configurations with sharp splits are generated. Then, generation of all of the possible TESs for the OTCs is presented. *Two rules* are developed for synthesizing the possible TESs for any OTC involving both sharp and sloppy splits. Formulas are derived to calculate the number of TESs for an *n*-component mixture. It is observed that there exist intrinsic uneven distributions of vapor and liquid flows between columns of the OTCs. The TESs provide the opportunities to redistribute the vapor and liquid flows between columns and thus improve column equipment designs of an OTC. Heuristics and a simple procedure have been approached to find an optimal TES.

1. Introduction

The design of a distillation system for a multicomponent separation can always start from those *traditional distillation configurations* (TDCs). However, there exists an inevitable separation inefficiency in a TDC due to thermodynamic irreversibility.[1] The separation inefficiency can be improved by using thermal couplings within a multicomponent distillation system. In certain cases, thermally coupled distillation systems can substantially reduce both energy consumption and capital costs compared to TDCs. Specifically, for ternary mixtures, the thermally coupled dividing-wall column (DWC)[2,3] has been used in many industrial separations, where 30−50% savings on both energy and capital costs has been achieved.[4,5]

A distinct feature of a thermally coupled configuration for a multicomponent distillation is that it can produce *thermodynamically equivalent structures* (TESs). For an *n*-component mixture, we illustrated that an *original thermally coupled configuration* (OTC) can be produced from a TDC by replacing those condensers and/or reboilers associated with submixtures of two or more components with thermal couplings.[6−8] The OTC can produce the TESs by rearrangement of the column sections.[7,8] For ternary mixtures, the *relationship* between the TDCs, their OTCs, and the possible TESs was illustrated in an earlier work.[7] It was shown that the well-known side rectifier (SR), side stripper (SS), DWC, and the more operable arrangements of the Petlyuk column[9] are the TESs of the corresponding OTCs. Those OTCs are produced from the TDCs with sharp and sloppy splits for a ternary mixture. It should be indicated that the relationships of the possible distillation configurations for ternary mixtures have not been fully appreciated in the previous works.[10−12] The understanding of the relationships of the possible distillation alternatives is useful to process engineers in the optimal design of a distillation system for a specific application. For example, the SR, SS, and DWC are the well-used ternary distillation systems in industries.[11,13]

The perceived relationship of the possible ternary distillation configurations has been extended to synthesize the possible thermally coupled configurations for four-component or more mixtures. For example, all of the functionally distinct thermally coupled configurations for quaternary mixtures have been synthesized from the TDCs.[8] A specific subspace of the TESs with side-column arrangements was also presented.[6,8] However, a distinct feature of a thermally coupled configuration for four-component or more mixtures is that it can produce a large number of possible TESs [e.g., Petlyuk-type fully coupled (FC)[1] configuration]. While one can say that all of the possible TESs for ternary mixtures have been known, it is not the same situation for four-component or more mixtures. There are a few works to find the possible TESs for four-component or more mixtures, mainly on the Petlyuk-type FC configurations. Agrawal[14] has drawn some specific arrangements for Petlyuk-type FC configurations for four- and five-component mixtures that are regarded as more operable arrangements with respect to the vapor transfers between columns. Caballero and Grossmann[15] presented a logic-based method to generate the possible TESs for a given sequence of tasks of a multicomponent distillation. Agrawal[16] also presented a method to draw TESs for Petlyuk-type FC configurations for four-component or more mixtures. However, it will be shown in this work that Agrawal's method[16] can only give part of all of the possible TESs for Petlyuk-type FC configurations for five-component or more mixtures.

While it is important to know how to generate all of the possible TESs for a thermally coupled configuration, a more important issue is to understand how the different arrangements of column sections in TESs will affect systems' design and operation. An earlier work to synthesize partially thermally coupled (PC) configurations for multicomponent distillations was presented.[6]

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Table 1. 14 Separation Sequences for a Five-Component Mixture

sequence no.	simple column sequence
1	ABCD/E → ABC/D → AB/C → A/B
2	ABCD/E → ABC/D → A/BC → B/C
3	ABCD/E → AB/CD → A/B → C/D
4	ABCD/E → A/BCD → B/CD → C/D
5	ABCD/E → A/BCD → BC/D → B/C
6	ABC/DE → D/E → A/BC → B/C
7	ABC/DE → D/E → AB/C → A/B
8	AB/CDE → A/B → CD/E → C/D
9	AB/CDE → A/B → C/DE → D/E
10	A/BCDE → BCD/E → BC/D → B/C
11	A/BCDE → BCD/E → B/CD → C/D
12	A/BCDE → BC/DE → B/C → D/E
13	A/BCDE → B/CDE → CD/E → C/D
14	A/BCDE → B/CDE → C/DE → D/E

Therein, we observed that, even though the difference of the capital costs among the TESs will not change the optimal PC system, there are still some differences between the TESs with regard to the column equipment designs. Most importantly, it will be shown in this work that *there exist intrinsic uneven distributions of vapor and liquid flows within columns of the OTCs. The rearrangements of the column sections in the TESs can provide the opportunity to redistribute the vapor and liquid flows of the OTC.* This will provide the opportunity for optimal design of a thermally coupled system not only for savings on energy and capital costs but also for improvement of the hydraulic performance of the distillation system.

The main objective of this paper is, on the one hand, to systematically synthesize all of the possible TESs for an *n*-component distillation and, on the other hand, to study their distinct features in terms of optimal column equipment designs. The work will first generate *the original PCs* from the traditional simple column (SC) configurations. Then, all of the possible *TESs* for the original PCs are formulated (TEPCs). In the fourth part, the lesson learned from the PCs has been extended to synthesize the TESs for any thermally coupled configurations involving both sharp and sloppy splits. An example is illustrated for the optimal design of TEPCs for a five-component separation. Finally, heuristics and a simple procedure are summarized for finding the optimal TESs for a multicomponent separation.

2. Generation of the Original Partially Thermally Coupled Configurations (OPCs) for an *n*-Component Distillation

For ternary and quaternary mixtures, we have illustrated that the generation of the TESs depends on the generation of the OTCs.[7,8] The generation of the OTCs depends on the generation of the TDCs. The generation of the TDCs depends on the identification of the distinct sets of intended individual splits that represent the functionally distinct separation sequences for a multicomponent distillation. As long as the distinct sets of intended individual splits are identified, the functionally distinct TDCs are determined from the functionally distinct separation sequences.[7,8]

For the SCs with only sharp splits, Thompson and King[17] presented an equation to calculate the number of such SCs for any *n*-component mixture. For example, for a five-component mixture, there are in total 14 SCs. Table 1 presents the 14 separation sequences of the SCs for a five-component distillation.

It is known that, in a SC for an *n*-component distillation, there are $n - 1$ simple columns.[1,17] Each simple column has a rectifying column section with a condenser and a stripping section with a reboiler. As a consequence, each SC has $2(n - 1)$ column sections as well as $2(n - 1)$ condensers and reboilers. It is observed that, among $2(n - 1)$ column sections in a SC, there are n column sections that produce the pure products from the condenser(s) and reboiler(s). Each of the n column sections is enriched with one of the components of the feed mixture, while the remaining $n - 2$ column sections do not produce the pure products but their condenser(s) and/or reboiler(s) are associated with the submixtures of two or more components. Thus, each of the $n - 2$ column sections is enriched with a submixture containing two or more components.[6,7] For each of the $n - 2$ column sections enriched with a submixture, there is an inevitable remixing. It is due to the condenser (reboiler) for supplying the liquid reflux (vapor boilup) for the column. This remixing will incur separation inefficiency. According to Petlyuk et al.,[1] this remixing can be avoided by eliminating the condenser or reboiler and interconnecting the columns by the two-way liquid and vapor streams, i.e., the thermal coupling streams. Each rectifying (stripping) section after elimination of its condenser (reboiler) will require the liquid reflux (vapor boilup) from its subsequent column. By doing so, it is expected that the irreversibility of the separation process is reduced and the separation efficiency is improved. One can expect that each thermal coupling will eliminate the remixing in a column section in a TDC. As a consequence, each thermal coupling will provide the improvement to the separation efficiency of the TDC. Thus, once a specific TDC for an *n*-component distillation is determined, its thermally coupled configuration is readily obtained by replacing all of the condensers and reboilers associated with submixtures with thermal coupling streams.[6−8]

As an example, Figure 1a illustrates the SC of separation sequence 9 in Table 1 for a five-component mixture. It is seen from Figure 1a that there are three column sections (i.e., $n - 2$) whose products are submixtures with two or three components. Column 1 has rectifying section 1 with condenser AB and stripping section 2 with reboiler CDE. Column 3 has stripping section 6 with reboiler DE. By replacement of the condenser(s) and reboiler(s) associated with submixtures with thermal couplings, the PC is produced as shown in Figure 1b. The PC of Figure 1b has exactly the same structural arrangements of the four columns as the SC of Figure 1a. We define it as the OPC with regard to the introduced thermal couplings for the SC. It will be shown in the next section that this OPC can produce *a certain number of TESs* by rearrangements of its column sections.

Obviously, each of the SCs can produce a unique OPC by directly replacing those condensers and/or reboilers associated with submixtures with thermal coupling streams. Thus, for any *n*-component mixture, the total number of OPCs is equal to the total number of SCs that can be calculated by the formula of eq 1 (Thompson and King[17]). The 14 OPCs for a five-component mixture

$$S_n = \frac{[2(n - 1)]!}{n!\,(n - 1)!} \qquad (1)$$

corresponding to the separation sequences in Table 1 are presented in Figure 2.

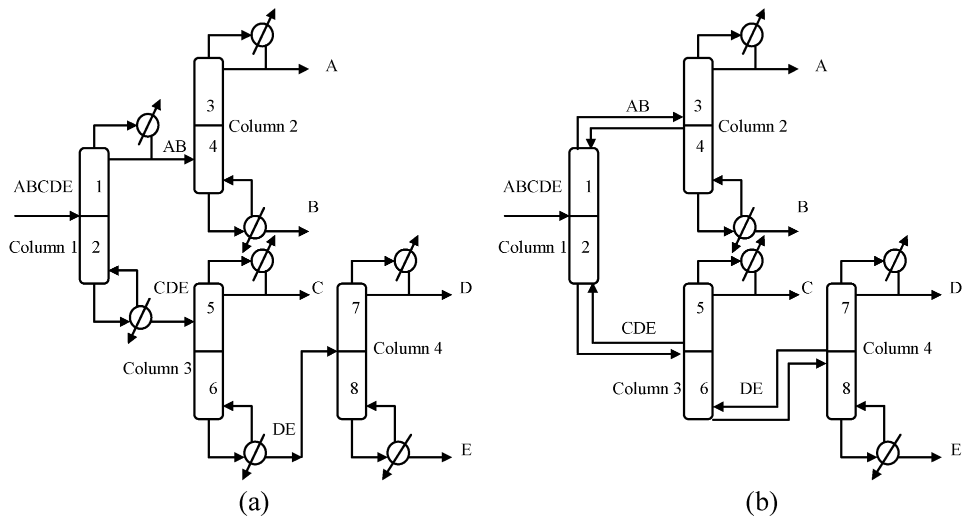

Figure 1. Five-component simple column configuration and its OTC.

There are some distinct features of the OPCs compared to the SCs. These distinct features are summarized as the following *observations*.

Observation No. 1. Each OPC has $n - 2$ thermal couplings associated with the $n - 2$ column sections enriched with submixtures. Each OPC has n condenser(s) and reboiler(s) at the n product column sections. In any OPC, the most volatile component is always produced from a condenser and the least volatile component is always produced from a reboiler; the intermediate volatility components are produced from either condenser(s) or reboiler(s).

Observation No. 2. Each OPC has $n - 1$ columns for the $n - 1$ individual splits in a separation sequence. Each column in an OPC has two column sections for a specific individual split, that is, the same counterpart of column sections for an intended individual split as in the SC.[7]

Observation No. 3. The elimination of a condenser (reboiler) of the SC will introduce a pair of vapor and liquid thermal coupling streams in the OPC. The vapor (liquid) flow is taken from the top (bottom) of the prior column and entering the intermediate location of its subsequent column. The liquid (vapor) flow is taken from the intermediate location of the subsequent column and entering the top (bottom) of the prior column. The former (eliminating a condenser) is defined as *a vapor feed thermal coupling* and the latter (eliminating a reboiler) as *a liquid feed thermal coupling*.

Observation No. 4. *The vapor and liquid flows of the thermal coupling streams in an OPC are always taken from a prior column of the two thermally linked columns*. For example, the vapor and liquid flows of the thermal coupling AB in the OPC of Figure 1b are taken from column 1 of the two thermally linked columns 1 and 2.

Most importantly, to see the changes of the vapor and liquid flows in the columns of the OPC, the relationships of the vapor and liquid flows for Figure 1a,b are presented in Table 2. Note that a similar table for each of the other configurations in Figure 2 is readily developed.

From Table 2, we have observed the following:

Observation No. 5. The first column with fresh feed in both the SC and its OPC has the same constraints on the vapor and liquid flows between the rectifying section and the stripping one. The vapor flow rate of the rectifying section is equal to that of the stripping one, and the liquid flow rate of the stripping section is greater than that of the rectifying one. However, for a column with a vapor feed thermal coupling (e.g., column 2 of Figure 1b), both the vapor and liquid flow rates of the rectifying section are greater than those of the stripping one. For a column with a liquid feed thermal coupling (e.g., columns 3 and 4 of Figure 1b), both the vapor and liquid flow rates of the rectifying section are smaller than those of the stripping one. This observation is valid for any OPC of an n-component mixture.

Observation No. 6. *There exist intrinsic uneven distributions of both vapor and liquid flows within the thermally linked columns in the OPCs. This will significantly affect the column equipment designs because the vapor and liquid flows are the dominant factors in determining the diameters of the columns, as well as the hydraulics*.

The above observations revealed that the replacement of the condensers and reboilers of the TDCs with thermal couplings will change the mass and heat transfers between the columns. The changes on mass and heat transfers between the columns can improve the separation efficiency in the OTCs, thus providing the potential to reduce both energy and capital costs. However, the thermally linked columns in the OTCs exist intrinsic uneven distributions of vapor and liquid flows between the columns. It will be shown in the next section that the vapor and liquid flows in the OPC can be redistributed in the TESs. *Although the TESs have the same nominal energy consumption as the OPC, they will provide the opportunity to mitigate the uneven distributions of vapor and liquid flows within the OPC. As a consequence, the TESs are capable of improving column equipment designs not only for capital cost reduction but also for higher hydraulic performance.*

3. Generation of the TEPCs

As stated above, in an OPC, each rectifying (stripping) section after elimination of its condenser (reboiler) will receive the liquid reflux (vapor boilup) flow from its subsequent column. From Figure 1b, it is seen that by replacement of condenser AB with the thermal coupling AB the liquid reflux in section 1 is supplied by its subsequent column 2. Both liquid refluxes of sections 1 and 3 are from condenser A in Figure 1b. Thus, a

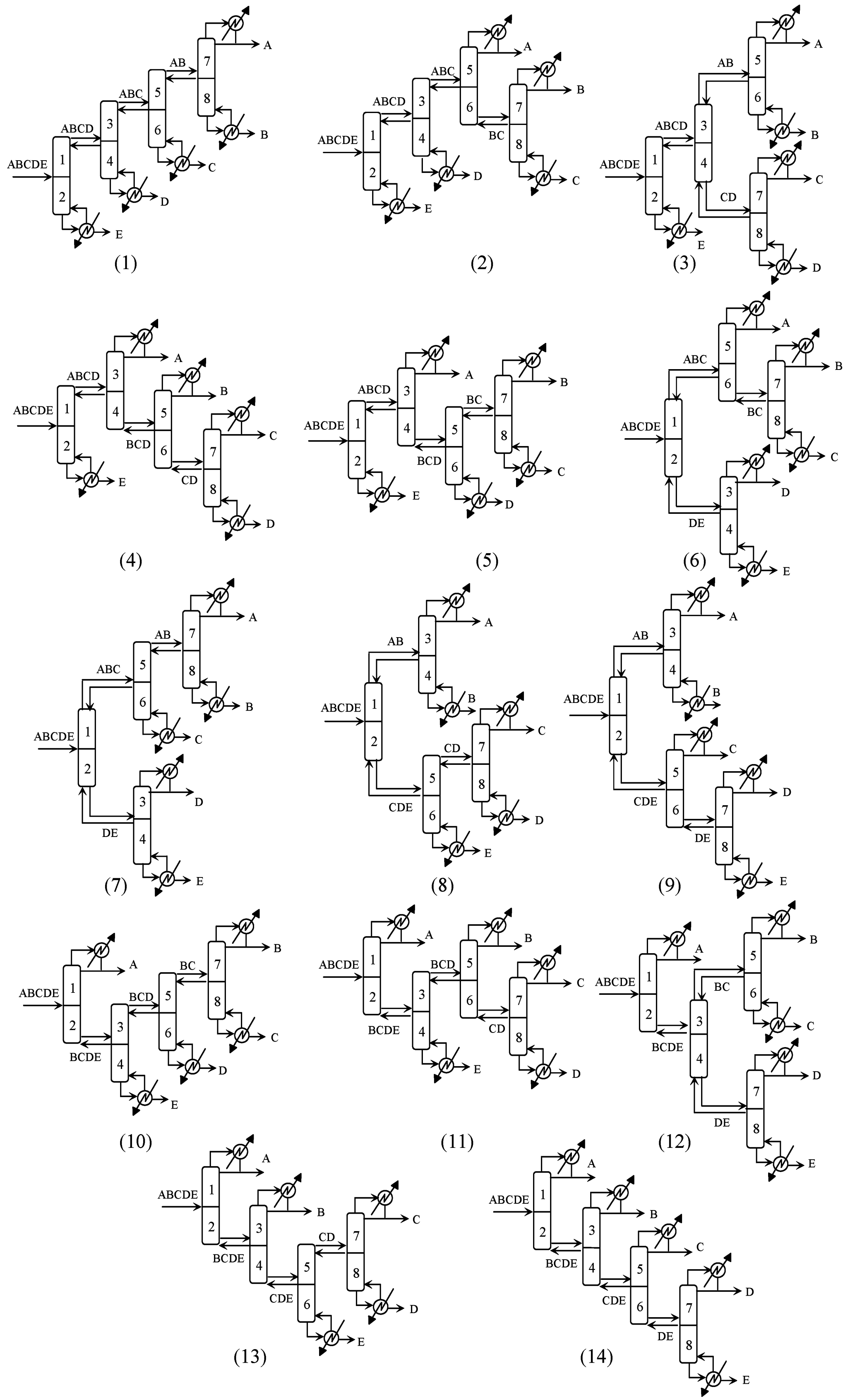

Figure 2. 14 OPCs for a five-component mixture.

structural degree of freedom is generated by the thermal coupling AB. The structural degree of freedom results in the fact that the two thermally linked rectifying sections 1 and 3 can be combined. They will receive the

Table 2. Equations and Constraints of Vapor and Liquid Flows of the SC and Its OPC in Figure 1[a]

column unit	SC configuration in Figure 1a equation	SC configuration in Figure 1a constraints	OPC configuration in Figure 1b equation	OPC configuration in Figure 1b constraints
column 1	$V_1 = V_2$		$V_1 = V_2$	
	$L_2 = L_1 + L_F$	$V_2 = V_1$	$L_2 = L_1 + L_F$	$V_2 = V_1$
	$V_1 = L_1 + L_{AB}$	$L_2 > L_1$		$L_2 > L_1$
	$L_2 = V_2 + L_{CDE}$			
column 2	$V_3 = V_4$		$V_3 = V_4 + V_1$	
	$L_4 = L_3 + L_{AB}$	$V_4 = V_3$	$L_3 = L_4 + L_1$	$V_4 < V_3$
	$V_3 = L_3 + L_A$	$L_4 > L_3$	$V_3 = L_3 + L_A$	$L_4 < L_3$
	$L_4 = V_4 + L_B$		$L_4 = V_4 + L_B$	
column 3	$V_5 = V_6$		$V_6 = V_5 + V_2$	
	$L_6 = L_5 + L_{CDE}$	$V_6 = V_5$	$L_6 = L_5 + L_2$	$V_6 > V_5$
	$V_5 = L_5 + L_C$	$L_6 > L_5$	$V_5 = L_5 + L_C$	$L_6 > L_5$
	$L_6 = V_6 + L_{DE}$			
column 4	$V_7 = V_8$		$V_8 = V_7 + V_6$	
	$L_8 = L_7 + L_{DE}$	$V_8 = V_7$	$L_8 = L_7 + L_6$	$V_8 > V_7$
	$V_7 = L_7 + L_D$	$L_8 > L_7$	$V_7 = L_7 + L_D$	$L_8 > L_7$
	$L_8 = V_8 + L_E$		$L_8 = V_8 + L_E$	

[a] The subscripts designate the vapor and liquid flows of column sections or the streams with the subgroups of the feed mixture.

Table 3. Thermal Couplings and Corresponding Movable Column Sections of the 14 OPCs in Figure 2

no. of OPCs	thermal couplings	movable column sections	no. of OPCs	thermal couplings	movable column sections
1	ABCD, ABC, AB	3, 5, 7	8	AB, CDE, CD	3, 6, 7
2	ABCD, ABC, BC	3, 5, 8	9	AB, CDE, DE	3, 6, 8
3	ABCD, AB, CD	3, 5, 8	10	BCDE, BCD, BC	4, 5, 7
4	ABCD, BCD, CD	3, 6, 8	11	BCDE, BCD, CD	4, 5, 8
5	ABCD, BCD, BC	3, 6, 7	12	BCDE, BC, DE	4, 5, 8
6	DE, ABC, BC	4, 5, 8	13	BCDE, CDE, CD	4, 6, 7
7	DE, ABC, AB	4, 5, 7	14	BCDE, CDE, DE	4, 6, 8

liquid refluxes from condenser A in the same column. In other words, section 3 of column 2 can be moved to the top of column 1. Similarly, when reboiler CDE of column 1 is replaced with thermal coupling CDE, the vapor boilup of column 1 is supplied by its subsequent column 3. Both vapor boilups of sections 2 and 6 are supplied by reboiler E in Figure 1b. The thermal coupling CDE produces *another structural degree of freedom* that the two thermally linked sections 2 and 6 can be combined into the same column or section 6 of column 3 can be moved to the bottom of column 1. The thermal coupling DE brings *the third structural degree of freedom* from which section 8 of column 4 can be moved to the bottom of column 3. *It is observed that, for any SC of an n-component mixture, the elimination of a condenser (reboiler) with a submixture in one column will make the rectifying section (stripping section) of its subsequent column movable*. Therefore, an OPC for an n-component distillation can have $n - 2$ *movable column sections*. They are designated by the $n - 2$ thermal couplings introduced into the $n - 2$ column sections enriched with submixtures of the SC. Table 3 presents the thermal couplings and corresponding movable column sections for the 14 OPCs in Figure 2.

Thus, in an OPC, each of the thermal couplings introduces a structural degree of freedom that will produce the *TESs. A TES is defined as a thermally coupled configuration that has the same individual splits and the same thermal couplings for the same submixtures, while it has different arrangements of the column sections than the OTC.*[7,8] The TESs can be generated by movement of the movable column sections designated in the OPC. The movement of the movable column sections in the OPC can be done in such a way that each time different structural degrees of freedom are used in rearrangements of the column sections.

In Figure 1b, the three thermal couplings AB, CDE, and DE generate three structural degrees of freedom that designate the three column sections 3, 6, and 8 movable. If we once move one column section of 3, 6, or 8, three TESs, as shown in parts a−c of Figure 3, respectively, will be produced. If we once move two column sections of (3, 6), (3, 8), or (6, 8), three other TESs, as shown in parts d−f of Figure 3, respectively, will be produced. If we simultaneously move all of the three movable column sections of 3, 6, and 8, a TES as in part g of Figure 3 will be produced.

On the basis of the identified movable column sections in Table 3, for each of the other OPCs in Figure 2, one can readily produce all of its TESs by movement of its movable column sections.

There are some distinct features of the TESs compared to the OPCs. These distinct features are summarized as the following observations.

Observation No. 7. Depending on the number of moved column sections, a column in the TESs can have a different number of column sections. However, the total number of columns in a TES is equal to the total number of columns in its OTC (not considering DWCs).

For TEPCs, the minimum number of sections in a column is 1 (a SS or a SR with one section) and the maximum number of sections in a column is n [subtract $n - 2$ SSs and/or SRs with one section from a total number of $2(n - 1)$ sections, e.g., Figure 3g]. In any cases, the two column sections for fresh feed must be in the same column. For example, a column in TEPCs of Figure 3 can have 1, 2, 3, 4, or 5 sections. Table 4 presents the distributions of the sections among the columns in the TEPCs of Figure 3, as well as the SC and OPC.

Observation No. 8. In any TESs, the n condenser(s) and reboiler(s) are always connected with the n product sections as in the OPC. Meanwhile, the most volatile component is always produced from a condenser, and the least volatile component is always produced from a reboiler; the intermediate volatility components are produced from either condenser(s) or reboiler(s).

Observation No. 9. The thermally linked rectifying (stripping) sections receiving the liquid (vapor) flows from the same condenser (reboiler) in an OPC can be combined into one same column in the TESs. When rectifying (stripping) sections of the subsequent columns are moved to the prior columns, the subsequent columns will become *SS (SR)*.

Observation No. 10. *When a column section is moved, the vapor and liquid flows of the thermal coupling streams between the two thermally linked columns in a TES will be different from those of its OPC. The vapor and liquid flows of the thermal coupling streams in a TES are taken from the subsequent column of the two thermally linked columns (see observation no. 4).*

For example, the vapor and liquid flows of thermal coupling AB in the OPC of Figure 1b are taken from the prior column 1 of the two thermally linked columns 1 and 2, while the vapor and liquid flows of thermal coupling AB in the TES of Figure 3a are taken from the subsequent column 2 of the two thermally linked columns 1 and 2. This means that the uneven distributions of the vapor and liquid flows in an OPC can be

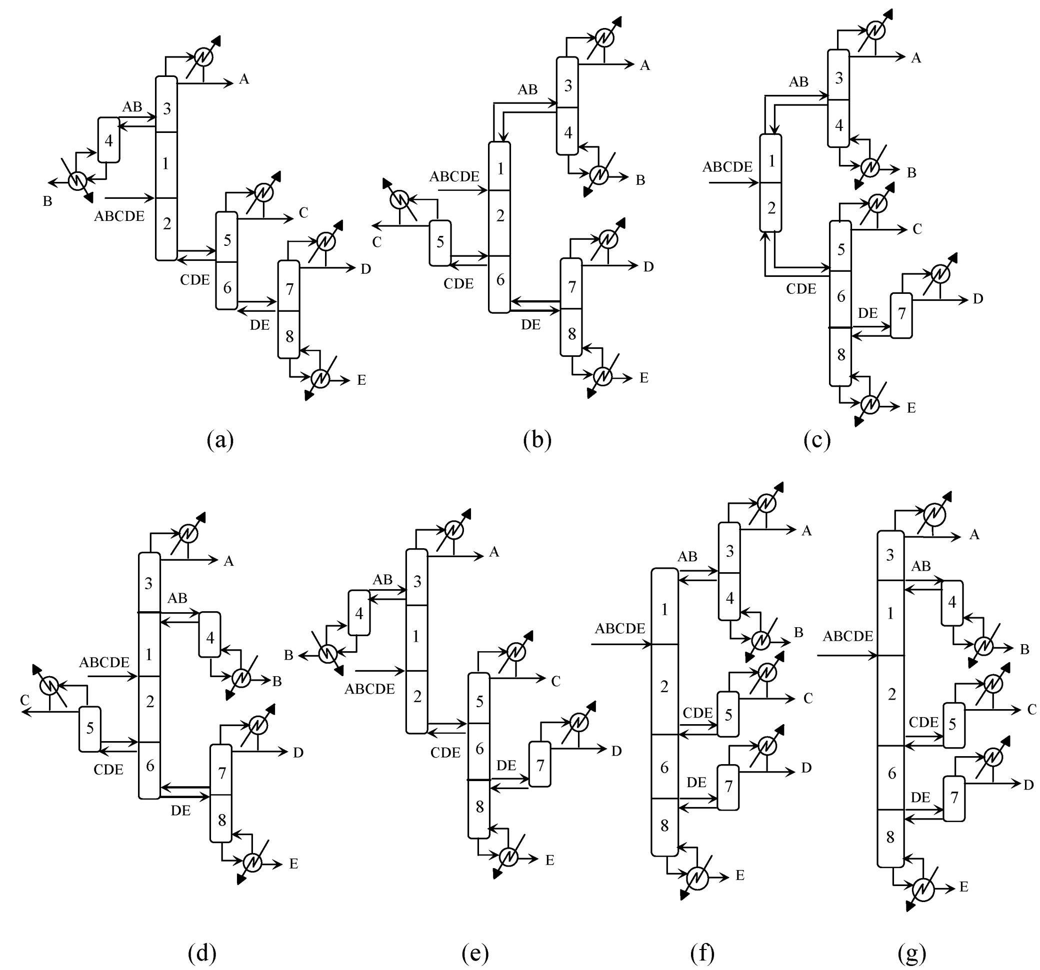

Figure 3. Thermodynamically equivalent arrangements of the OPC in Figure 1b.

Table 4. Distributions of the Column Sections in TEPCs of Figure 3 and the SC and OPC

configuration	moved column section(s)	column section distribution: column 1	column 2	column 3	column 4	total
SC		2	2	2	2	8
OPC	none	2	2	2	2	8
3a	3	3	1	2	2	8
3b	6	3	2	1	2	8
3c	8	2	2	3	1	8
3d	3, 6	4	1	1	2	8
3e	3, 8	3	1	3	1	8
3f	6, 8	4	2	1	1	8
3g	3, 6, 8	5	1	1	1	8

redistributed by rearrangement of the column sections in the TESs.

Observation No. 11. *The flow directions of the two-way thermal coupling streams between the two thermally linked columns in a TES will be opposite to those of its OPC. When a rectifying (stripping) section is moved, the vapor (liquid) flow is from the subsequent column to the prior column and the liquid (vapor) flow is from the prior column to the subsequent column (see observation nos. 3 and 4).*

This will change the pressure constraints between the columns of the TESs.[18] This is because the pressure of the column withdrawing a vapor flow is expected to be a little higher than that of the column receiving the vapor flow in a thermally coupled system in order to avoid the use of expensive compressors.[10]

Observation No. 12. The TES of Figure 3g, which is produced by simultaneously moving all of the movable column sections of the OPC in Figure 1b, has some special features: (1) A main column with a fresh feed is used to produce the most volatile component from the top condenser and the least volatile component from the bottom reboiler. (2) Each of the intermediate volatility products is produced from a side column, either a SS or a SR. Each of the OPCs in Figure 2 can produce a unique TES in which the side columns are SSs and/or SRs.

The above observations revealed that the rearrangements of the column sections in the TESs provide the opportunities for optimal design and operation of the thermally coupled distillation systems. Specifically, column sections with similar vapor and liquid flow rates can be combined into the same column in the TES such that each column could have a uniform diameter. This will not only mitigate the uneven distributions of the vapor and liquid flows between the columns in the OPC, thus improving the hydraulic performance, but also improve column equipment designs for capital cost savings. Moreover, some specific TESs can be distinguished in which the vapor flows of the thermal coupling streams can flow from higher pressure columns to lower pressure ones. Such specific TESs had once been illustrated for Petlyuk-type FC configurations and were called more operable fully thermally coupled configurations.[9,14]

In the next section, the synthesis of the TESs for any thermally coupled configurations of an *n*-component mixture is presented.

4. TESs of Thermally Coupled Configurations for an *n*-Component Distillation

It was shown that an OTC can be generated from any TDC involving both sharp and sloppy splits for an *n*-component mixture.[8,19] Then, it is a problem of paramount importance to systematically produce all of the possible TESs for any OTC. To do so, *two rules* have been developed for the synthesis of all TESs for any thermally coupled configuration of an *n*-component mixture.

As discussed earlier, in any SC for an *n*-component distillation, $n - 2$ condenser(s) and/or reboiler(s) associated with submixtures of two or more components can be eliminated. Thus, $n - 2$ thermal couplings for a SC of an *n*-component distillation can be introduced. This means that there will be $n - 2$ *structural degrees of freedom* in a PC. This also means that there are $n - 2$ column sections in a PC that are movable among the columns. The following formula of eq 2 is derived for calculation of the number of TEPCs (TPC_n) for an *n*-component mixture ($n \geq 3$)

$$\mathrm{TPC}_n = \sum_{i=0}^{n-2} C_{n-2}^{i} = 2^{n-2} \quad (2)$$

where $C_{n-2}^{0} = 1$ designates the OPC without movement of column sections (e.g., Figure 1b), C_{n-2}^{i} ($i = 1, n - 3$) designates the number of TESs by once moving *i* column sections (e.g., parts a–c or parts d–f in Figure 3), and $C_{n-2}^{n-2} = 1$ designates the side-column TES by simultaneously moving all of the $n - 2$ movable column sections (e.g., Figure 3g).

From the above derivation, it is clear that the number of TESs of a thermally coupled distillation configuration depends on the number of structural degrees of freedom with respect to the introduced thermal couplings. Thus, rule 1 for synthesis of TESs for a thermally coupled configuration is developed as follows:

Rule 1. *Number of Structural Degrees of Freedom.* *The number of structural degrees of freedom in a thermally coupled distillation configuration is equal to the number of thermal couplings introduced into its TDC. Each of the structural degrees of freedom corresponds to one of the thermal couplings.*

As discussed above, the generation of the TESs for a thermally coupled configuration depends on the movable column sections designated by the structural degrees of freedom. For any PC in Figure 2, each thermal coupling introduces a structural degree of freedom that designates a *unique* movable column section (see Table 3). It is seen that, in any PC in Figure 2, a thermal coupling must be connected with one end of a column. In other words, a submixture with two or more components in PCs must transfer from one end of a column to an intermediate location of another column. However, in thermally coupled configurations involving sloppy splits, some of the submixtures with two or more components might transfer between intermediate locations of two columns. For example, among all of the functionally distinct thermally coupled configurations for quaternary mixtures,[8] there are four configurations in which there is an intermediate submixture BC transferring between intermediate locations of two columns, which are illustrated in Figure 4. For such an intermediate submixture, the introduced thermal coupling will make a pair of column sections of its subsequent column movable. However, this pair of movable column sections must be moved simultaneously in rearrangements of the column sections. Thus, it will also introduce one structural degree of freedom from such a thermal coupling of an intermediate submixture. We call it *a counterpart of movable column sections* corresponding to the structural degree of freedom from a thermal coupling of an intermediate submixture. Moreover, if an intermediate volatility product is produced from an intermediate location of a column without a heat exchanger (e.g., product C in Figure 4a), then the two column sections coproducing this intermediate volatility product must be moved together (e.g., column sections 8 and 9 coproducing product C). In other words, a pair of column sections coproducing an intermediate volatility product must stay together in rearrangements of column sections during the synthesis of the TESs. For example, in a functionally distinct thermally coupled configuration of Figure 4d, the thermal coupling of the intermediate submixture BC will introduce a structural degree of freedom that designates a counterpart of movable column sections 9 and 10. However, column sections 8 and 9 must stay together for coproducing the intermediate volatility product B, and column sections 10 and 11 must stay together for coproducing the intermediate volatility product C. Therefore, these four column sections must be moved simultaneously in producing the TESs. Note that when using the structural degree of freedom of the pair of movable column sections 8 + 9 and 10 + 11 alone, the connected sections 7 and 12 should be moved together. Thus, rule 2 for the synthesis of the TESs for a thermally coupled configuration is developed as follows:

Rule 2. *Number of Movable Column Sections.* *Each of the thermal couplings in a thermally coupled distillation configuration designates a movable column section (or a counterpart of movable column sections). The number of movable column sections (including the counterparts of movable column sections) in a thermally coupled configuration is equal to the number of the structural degrees of freedom. In other words, the number of movable column sections (including the counterparts of movable column sections) in a thermally coupled distillation configuration is equal to the number of thermal couplings introduced into its TDC.*

For a Petlyuk-type FC configuration of an *n*-component mixture, there are a total of $n(n + 1)/2$ distinct subgroups including the feed and *n* products.[1] Thus, $(n - 2)(n + 1)/2$ thermal couplings exist for the $(n - 2)(n + 1)/2$ distinct submixtures with two or more components in a Petlyuk-type FC. Therefore, *there are a total of $(n - 2)(n + 1)/2$ structural degrees of freedom in a Petlyuk-type FC configuration for the generation of the TESs*. The number of TESs for a Petlyuk-type FC of an *n*-component distillation (TFC_n) can be calculated by the formula given in eq 3.

$$\mathrm{TFC}_n = \sum_{i=0}^{(n-2)(n+1)/2} C_{(n-2)(n+1)/2}^{i} = 2^{(n-2)(n+1)/2} \quad (3)$$

Table 5 presents the number of TESs for a PC and a Petlyuk-type FC with different numbers of components in the feed mixture. From Table 5, it is seen that the earlier work for generation of the TESs for the Petlyuk-type FC has produced only part of all possible alternatives for five-component or more mixtures.[16]

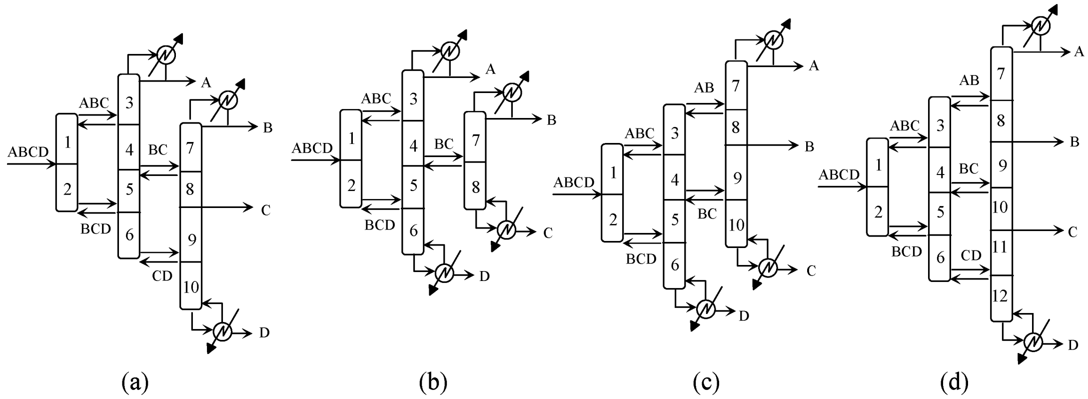

Figure 4. OTCs involving an intermediate submixture for quaternary mixtures.

Table 5. Number of TESs for a PC and a Petlyuk-type FC Configuration of an *n*-Component Mixture

no. of components n	no. of thermal couplings in a PC $n-2$	no. of TESs for a PC 2^{n-2}	no. of thermal couplings in a FC $(n-2)(n+1)/2$	no. of TESs for a FC $2^{(n-2)(n+1)/2}$
3	1	2	2	4
4	2	4	5	32
5	3	8	9	512
6	4	16	14	16384
7	5	32	20	1048576
8	6	64	27	134217728
9	7	128	35	34359738368
10	8	256	44	17592186044416

Table 6. Thermal Couplings, Movable Column Sections, and Number of TESs for the OTCs in Figure 4

configuration	thermal couplings	movable column sections	no. of TESs
4a	ABC	3	16
	BCD	6	
	CD	10	
	BC	**7, 8 + 9**	
4b	ABC	3	8
	BCD	6	
	BC	**7, 8**	
4c	ABC	3	16
	BCD	6	
	AB	7	
	BC	**9 + 8, 10**	
4d	ABC	3	32
	BCD	6	
	AB	7	
	CD	12	
	BC	**9 + 8, 10 + 11**	

It is clear that, for any thermally coupled configuration of an *n*-component distillation, as long as the number of thermal couplings (NTC) is determined, the number of all of its possible TESs (TTC_n) is readily calculated by the formula given in eq 4.

$$\mathrm{TTC}_n = \sum_{i=0}^{\mathrm{NTC}} C_{\mathrm{NTC}}^{i} = 2^{\mathrm{NTC}} \qquad (4)$$

For example, the numbers of TESs for the OTCs in parts a–d of Figure 4 are 16, 8, 16, and 32, respectively. Moreover, as long as the movable column sections are identified, the generation of all of the TESs can be systematically done by movement of the movable column sections. For example, the movable column sections for the OTCs in parts a–d of Figure 4 are identified in Table 6 (boldface for the intermediate submixture). As an example, Figure 5 presents all of the 16 TESs for the OTC of Figure 4a. Part 1 of Figure 5 is the OTC without sections movement. Parts 2–5 of Figure 5 are obtained by once using one structural degree of freedom. Parts 6–11 of Figure 5 are obtained by once using two structural degrees of freedom. Parts 12–15 of Figure 5 are obtained by once using three structural degrees of freedom. Finally, part 16 of Figure 5 is obtained by simultaneously using all of the four structural degrees of freedom. Like Figure 3g, part 16 of Figure 5 is the thermodynamically equivalent side-column structure of the OTC in Figure 4a, which was obtained by simultaneous movement all of the movable column sections. A special subspace of such thermodynamically equivalent side-column arrangements of thermally coupled configurations had been formulated for four- and five-component mixtures.[6,8]

5. Example for the Optimal Design of TEPCs

For PCs of an *n*-component distillation, the total number of TEPCs for all of the OPCs can be calculated by the formula given in eq 5.

$$\mathrm{TEPC}_n = S_n \times \mathrm{TPC}_n = \frac{[2(n-1)]!}{n!(n-1)!} \times 2^{n-2} \qquad (5)$$

Table 7 presents the number of OPCs, as well as the number of the total TEPCs generated from the SCs for feed mixtures with different numbers of components. Obviously, the TEPCs have formulated a new space of the thermally coupled systems for the well-known SCs for the optimal design of multicomponent distillation systems.

The significant criteria to evaluate the performance of a distillation system are of three aspects: the energy consumption, the capital investment, and the operability. The different arrangements of the column sections in the TESs will affect both the column equipment designs and operation of the thermally coupled systems. Even though the TESs have nominally the same energy

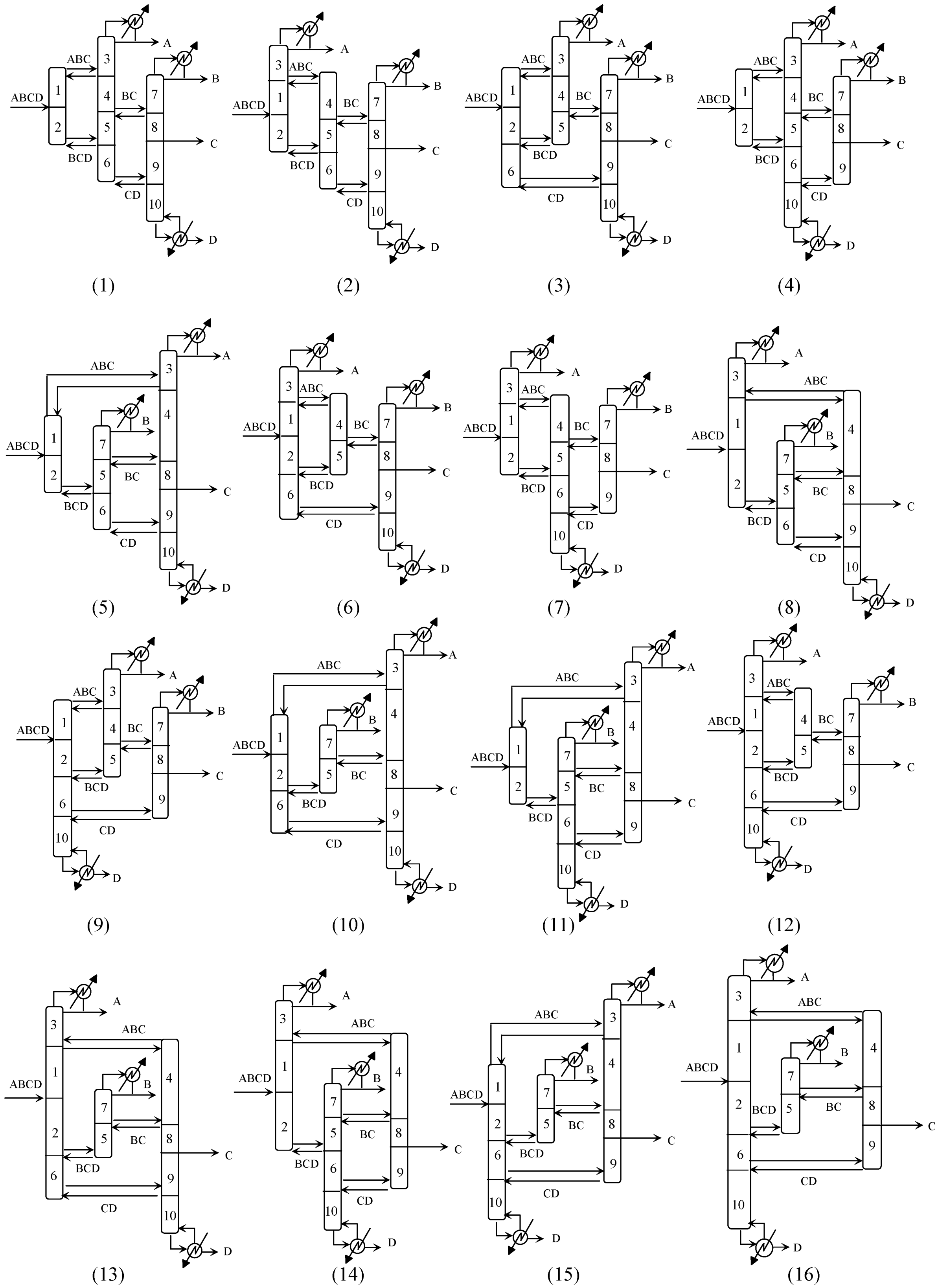

Figure 5. 16 TESs of the OTC in Figure 4a.

consumption, their capital costs and operability could be very different. The diameters and heights of the columns are changing among the TESs of a thermally coupled configuration. These two equipment parameters are of paramount importance in determining the capital cost of a column. The diameter is related to the vapor flow rates in the column sections within a unit, while the height of a column is related to the number of column trays (or height of packings) within the unit. As for the operability, the vapor flow directions of the thermal coupling streams are changing in the TESs (see observation no. 11). This will change the constraints on the pressures between the columns in the design of a thermally coupled system.[18]

Table 7. Number of TEPCs Generated from the SCs for an *n*-Component Mixture

no. of components *n*	no. of SC configurations	no. of OPC configurations	no. of total TEPC configurations
3	2	2	4
4	5	5	20
5	14	14	112
6	42	42	672
7	132	132	4224
8	429	429	27456
9	1430	1430	183040
10	4862	4862	1244672
11	16796	16796	8599552

Table 8. Design Results for the OPC of Figure 1b[a]

parameters	column 1	column 2	column 3	column 4
V (kmol/h)	768.63 (1)	2185.07 (3)	702.75 (5)	221.52 (7)
L (kmol/h)	566.72 (1)	2061.25 (3)	531.78 (5)	168.54 (7)
V_a (kmol/h)	768.63 (2)	1416.44 (4)	1471.38 (6)	1692.90 (8)
L_a (kmol/h)	1067.12 (2)	1494.54 (4)	1598.90 (6)	1767.44 (8)
N_{rt}	13 (1)	61 (3)	26 (5)	25 (7)
N_{st}	16 (2)	50 (4)	19 (6)	29 (8)

[a] Numbers in parentheses refer to column sections in Figure 1b. V_a, L_a = vapor and liquid flows in stripping sections. N_{rt}, N_{st} = number of column trays in rectifying and stripping sections.

To examine how the TESs will affect the column equipment designs, an example for the optimal design of the TEPCs for a five-component mixture is presented. This example was previously used for economic comparisons between all of PCs and the SCs.[6,7] In our previous studies,[6,7] the PC corresponding to the separation sequence 9 in Table 1 has been found to be the best one among the 14 PCs.[6] It was also found that the SC corresponding to the separation sequence 9 in Table 1 is the best one among the 14 SCs.[6] This SC and its OPC were illustrated in parts a and b of Figure 1, respectively. According to previous studies,[6] the optimal PC can have 16.7% more energy savings than the optimal SC.

As observed in part 2, there exist intrinsic uneven distributions of vapor and liquid flows between the columns of the OPC. It can be expected that the difference of the vapor flows among the column sections in the OPC will depend on the feed conditions, i.e., the relative volatilities and compositions of the feed components. In some cases, if the vapor flows between the rectifying section and the stripping one within a column are dramatically different, then there will be difficulty designing the column to cope with the vapor flow distribution. However, because some of the column sections in the OPC are movable, there is an opportunity to rearrange the column sections to cope with the uneven distributions of the vapor and liquid flows in the TESs. The rearrangements of the column sections can be done in such a way that the sections with similar vapor flow rates are combined into one column. By doing so, the columns in a TES can have relatively uniform diameters. *Most importantly, some column sections with small vapor flow rates can stand as small side columns.* This will not only contribute to the column equipment designs concerning the capital costs but also improve the hydraulic performance of the column equipment.

For this example problem, the design results for the OPC of Figure 1b are presented in Table 8. For details concerning the calculations, one can refer to our previous works.[7,18] From Table 8, it is seen that in the OPC of Figure 1b, except column 1, each of the other three columns has a dramatic difference of the vapor and liquid flows between its rectifying section and the stripping one. For column 2, the vapor flow rate in the rectifying section is 54.3% more than that of the stripping one. For columns 3 and 4, the vapor flow rates in the stripping section are 109.4% and 664.2% more than those of the rectifying one, respectively. Table 9 presents the rearrangements of the column sections in the TESs in Figure 3 for the OPC in Figure 1b. To examine the distributions of the vapor flows within the columns of the TESs, the maximum and minimum vapor flows in the columns of the TESs are presented in Table 10.

From the results in Tables 9 and 10, it is seen that each of the TESs in Figure 3a–e has either sections 5 and 6 or sections 7 and 8 or both together in one column. As discussed above, because these two pairs of sections have dramatic differences of vapor and liquid flows, it will be difficult for column equipment designs if they stay together. In the remaining two TESs of parts f and g of Figure 3, the TEPC of Figure 3f is identified as the optimal arrangement of the column sections among the units. According to the relative volatility of the feed mixture, the A/B split is difficult and needs a large number of column stages (see Table 9). Moreover, the vapor flow rate of section 3 is much higher than that of section 1; thus, it is not suitable to move section 3 to section 1. Therefore, sections 3 and 4 should stay together as a stand-alone column. It can be designed as *a swedge column* with different diameters for the rectifying section 3 and the stripping section 4. This arrangement is also considering the heuristics for sequencing multicomponent distillations; i.e., difficult separations should be performed last.[20] Then, two *small SR columns* are used to produce the intermediate volatility products C and D. On the basis of the number of column trays as well as the vapor flow rates of sections 5 and 7 in Table 10, these *two small SRs* can have much lower capital costs than any other possible arrangements. Finally, the main column with fresh feed has four sections of 1, 2, 6, and 8. The main column can also be designed as *a swedge column* according to the vapor flows of its column sections. Sections 1 and 2 can have the same diameter because of the same vapor flows of the two sections, and sections 6 and 8 can have another same diameter because of the similar vapor flows of the two sections. It is also seen that the vapor flows of the thermal coupling streams unidirectionally transfer among the columns in the TES of Figure 3f.

6. Heuristics and a Procedure To Determine the Optimal TESs

On the basis of the observations presented in sections 2 and 3, as well as the results from the above example problem, the following *heuristics* are proposed to identify the optimal TESs.

Heuristic 1. Column sections with similar vapor and liquid flow rates should be combined in a thermally coupled distillation configuration.

Heuristic 2. Column sections with substantially different vapor and liquid flow rates should not stay together in an original thermally coupled distillation configuration.

Heuristic 3. Column sections with substantially different vapor and liquid flow rates should not be combined in a TES.

Heuristic 4. Whenever possible, those column sections with small vapor and liquid flows should be arranged as stand-alone side columns.

Table 9. Column Sections and Number of Column Trays of the TESs in Figures 1b and 3

	column 1		column 2		column 3		column 4	
figure	section(s)	N_t	section(s)	N_t	section(s)	N_t	section(s)	N_t
1b	1 + 2	29	3 + 4	111	5 + 6	45	7 + 8	54
3a	3 + 1 + 2	90	4	50	5 + 6	45	7 + 8	54
3b	1 + 2 + 6	48	3 + 4	111	5	26	7 + 8	54
3c	1 + 2	29	3 + 4	111	5 + 6 + 8	74	7	25
3d	3 + 1 + 2 + 6	109	4	50	5	26	7 + 8	54
3e	3 + 1 + 2	90	4	50	5 + 6 + 8	74	7	25
3f	1 + 2 + 6 + 8	77	3 + 4	111	5	26	7	25
3g	3 + 1 + 2 + 6 + 8	138	4	50	5	26	7	25

Table 10. Maximum and Minimum Vapor Flows in Column Units of the TESs

	column 1		column 2		column 3		column 4	
figure	V_{max}	V_{min}	V_{max}	V_{min}	V_{max}	V_{min}	V_{max}	V_{min}
1b	768.63	768.63	2185.07	1416.44	1471.38	702.75	1692.90	221.52
3a	2185.07	768.63	1416.44	1416.44	1471.38	702.75	1692.90	221.52
3b	1471.38	768.63	2185.07	1416.44	702.75	702.75	1692.90	221.52
3c	768.63	768.63	2185.07	1416.44	1692.90	702.75	221.52	221.52
3d	2185.07	768.63	1416.44	1416.44	702.75	702.75	1692.90	221.52
3e	2185.07	768.63	1416.44	1416.44	1692.90	702.75	221.52	221.52
3f	1692.90	768.63	2185.07	1416.44	702.75	702.75	221.52	221.52
3g	2185.07	768.63	1416.44	1416.44	702.75	702.75	221.52	221.52

Heuristic 5. With all similar vapor and liquid flows among the column sections, the arrangements of the column sections in which the vapor flows of the thermal coupling streams unidirectionally transfer between the columns in a TES are preferred.

With the above heuristics, a simple procedure to design the optimal TESs can be summarized as follows:

Step 1. Design the OTC to give the operating and equipment parameters, like the results in Table 8 for Figure 1b. This can be done based on shortcut methods.[18]

Step 2. Identify the movable column sections in the OTC that can be rearranged to produce TESs. For example, there are three movable column sections of 3, 6, and 8 in Figure 1b that can produce the TEPCs shown in Figure 3.

Step 3. Identify the column sections in the OTC that are not suitable to stay together based on a comparison of the vapor and liquid flows in the column sections of the OTC. For example, in Figure 1b, column sections 5 and 6 and column sections 7 and 8 are not suitable to stay together because of the dramatic differences of their vapor and liquid flows.

Step 4. Identify the movable column sections in the OTC that are not suitable to be combined with the corresponding sections of prior columns based on a comparison of the vapor and liquid flows in the OTC. For example, in Figure 1b, the movable section 3 is not suitable to be combined with section 1 because of the dramatic differences of their vapor and liquid flows.

Step 5. Arrange those column sections with small vapor and liquid flows as stand-alone side columns. For example, column sections 5 and 7 in Figure 1b can be arranged as small side columns because of the small vapor and liquid flow rates.

Step 6. For the TESs remaining after steps 3−5, determine the optimal TESs by simultaneously considering the operability of the TESs, for instance, the vapor flow directions of the thermal coupling streams.

Step 7. Determine the specific column equipment designs in the obtained optimal TESs in terms of diameters and heights of the column units.

On the basis of this procedure, the optimal thermally coupled distillation systems can be identified with respect to energy consumption, capital cost, and operability. However, the final design and fabrication of the column equipment for a thermally coupled distillation system in a specific industrial application will be case-based. The physicochemical and thermodynamic properties of the multicomponent mixture, the hydraulics, and other material issues should further be considered.

7. Conclusions

The TDCs have intrinsic separation inefficiency in terms of mass and heat transfers for a multicomponent distillation. The separation efficiency of the TDCs can be improved by using thermal couplings that produce the OTCs. The thermal couplings will introduce structural degrees of freedom into the OTCs that produce the TESs. The thermally coupled distillation systems can save both energy and capital costs thanks to the improvement of the separation efficiency.

The OTCs have intrinsic uneven distributions of vapor and liquid flows between columns. A distinct feature of an OTC is that it has structural degrees of freedom to rearrange its column sections. *The number of structural degrees of freedom in an OTC is equal to the number of thermal couplings introduced into its TDC. The structural degrees of freedom in a thermally coupled configuration are related to those movable column sections designated by the introduced thermal couplings*. The rearrangements of the column sections can produce TESs. The TESs provide the opportunity to redistribute the vapor and liquid flows between the columns of the OTCs. This will improve not only column equipment designs but also the hydraulic performance and operability of a thermally coupled distillation system.

In this paper, the synthesis and optimal design of thermodynamically equivalent thermally coupled distillation systems for multicomponent separations is studied. Systematic generation of both the OPCs and their TEPCs for the SCs is presented first. This provides a new space of the thermally coupled configurations for the well-studied SCs of an *n*-component distillation. Systematic synthesis of all of the possible TESs for any OTC involving both sharp and sloppy splits is approached by the *two rules* developed. The formulas are derived to calculate the number of TESs for the OTCs of an *n*-component mixture. An example of a five-component separation has demonstrated the optimal design of the TESs with respect to column equipment designs. Finally, the heuristics and a procedure are presented to find an optimal TES for a specific application.

From this study, we learned that the essence to design an optimal thermally coupled distillation system for a multicomponent separation is to determine the optimal arrangement of the column sections among the TESs. This will not only ensure the savings on energy and capital costs but also improve the hydraulic performance and operability of the thermally coupled distillation systems.

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