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Systematic Synthesis of Functionally Distinct New Distillation Systems for Five-Component Separations

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Abstract

The predefinition of all of the possible alternatives to formulate a complete space is the precondition in searching an optimal alternative for a specific application in process synthesis. In this paper, the synthesis of the functionally distinct distillation systems for five-component separations is presented. First, all of the possible first splits for the feed mixture are identified. Then, for each of the first splits, all of its feasible separation sequences are identified. Finally, all of the distinct separation sequences for the feed mixture are determined. In total, 569 functionally distinct separation sequences have been identified for five-component separations. These functionally distinct separation sequences can then be used to produce the functionally distinct distillation systems for the feed mixture. They include the functionally distinct thermally coupled configurations, as well as the thermodynamically equivalent structures. All the produced alternatives can formulate the complete space of the feasible configurations for five-component distillations. This guarantees that the global optimal distillation system can be obtained for the five-component separations by the optimisation methods.

Keywords: synthesis, distinct separation sequence, thermal coupling, new distillation system, five-component separation

1. Introduction

Process synthesis and design in industrial practice showed that “The quality of the solution is heavily dependent on the quality and completeness of the process alternatives under consideration. *If the optimum alternative is not predefined it will not be found*.” (Kaibel & Schoenmakers, 2002). For ternary distillations, new distillation systems have been formulated through thermal couplings by considering both sharp and sloppy splits in a separation sequence. Specifically, the thermally coupled dividing-wall column (DWC) has been successfully used in many industrial applications for savings of both energy and capital costs. While one can say that all of the possible new thermally coupled distillation systems for ternary separations have been known, it’s not the same situation for four or more component separations.

Traditional works on process synthesis for multicomponent distillations have been mainly on the conventional simple column sequences with sharp splits. Specifically, the earlier works have focused on either optimum sequencing the simple columns since the work by Heaven (1969) or finding the optimal heat-integrated simple column sequences since the work by Rathore et al. (1974), where a considerable works have been done for five-component separations. On the other hand, separation problems involving five or more component mixtures are often encountered in petrochemical and other process industries. However, the publications so far have generated only part of all of the functionally distinct systems for five-component distillations (Agrawal, 2003; Rong et al., 2003a).

The works on synthesis of all of the feasible configurations for ternary and quaternary mixtures have progressively contributed to formulate a complete space from which an optimal system for a specific application can be searched. Therefore, synthesis of all of the feasible configurations for five-component mixtures will also be paramount importance for providing a complete space for optimal design in a specific application. However, it is a much complex task than either ternary or quaternary separations because of the large number of possible schemes for a five-component separation. The objective of this work is to develop a systematic procedure to predefine all of the functionally distinct distillation systems for five-component separations. The procedure is based on identifying the functionally distinct separation sequences by simultaneously considering both sharp and sloppy splits in the separation sequences.

2. Generation of All Functionally Distinct Separation Sequences for Five-Component Mixtures

For ternary and quaternary mixtures, it was found that all of the functionally distinct distillation configurations were produced from the functionally distinct separation sequences (Rong et al., 2003b). All of the functionally distinct separation sequences are identified by formulating the distinct sets of intended individual splits. All of the distinct intended individual splits are generated by three different types of splits: *the sharp split, the symmetric sloppy split, and the asymmetric sloppy split*. *A functionally distinct separation sequence* is defined as a separation sequence where at least one of its individual splits is different from the other possible separation sequences (Rong et al. 2003b).

If we simultaneously consider the three different types of splits for a multicomponent mixture, then there can produce in total n(n-1)/2 *first splits* for an n-component mixture (Rong et al., 2003b). For a five-component separation, there are ten different first splits which are presented in Table 1. Each first split will generate two subgroups, the one with the most volatile component A is called *Light Subgroup*(LS), and another with the least volatile component E is called *Heavy Subgroup* (HS). These two subgroups will determine the total number of distinct separation sequences generated from that first split. Therefore, if we identify the feasible separation sequences for each of the first splits, then the total number of the distinct separation sequences for the feed mixture will be determined. It is known that a five-component mixture can generate the following distinct submixtures that one needs further to determine their intended individual splits (ABCD, BCDE, ABC, BCD, CDE). In order to formulate the distinct separation sequences for the feed mixture, we need first to formulate the distinct separation sequences for these distinct submixtures. It is known that each of the submixtures can follow different sequences to approach its single components. However, during formulating a functionally distinct separation sequence, each distinct submixture with ternary or more components can only designate one intended individual split in a separation sequence. Table 2 presents the distinct sequences for each of the three ternary submixtures. Table 3 presents the distinct separation sequences for each of the two quaternary submixtures.

Table 1. First splits for a five-component separation

First Splits		Distributed Middle Component(s)	Light Subgroup	Heavy Subgroup	Number of Distinct Sequences
1	A/BCDE	none	A	BCDE	22
2	AB/CDE	none	AB	CDE	3
3	ABC/DE	none	ABC	DE	3
4	ABCD/E	none	ABCD	E	22
5	AB̲CDE	B	AB	BCDE	22
6	ABC̲DE	C	ABC	CDE	9
7	ABCD̲E	D	ABCD	DE	22
8	AB̲C̲DE	BC	ABC	BCDE	66
9	ABC̲D̲E	CD	ABCD	CDE	66
10	AB̲C̲D̲E	BCD	ABCD	BCDE	334

Table 2. Distinct separation sequences for ternary submixtures

1	A/BC→B/C	1	B/CD→C/D	1	C/DE→D/E
2	AB/C→A/B	2	BC/D→B/C	2	CD/E→C/D
3	AB̲C→A/B→B/C	3	BC̲D→B/C→C/D	3	CD̲E→C/D→D/E

Table 3. Distinct separation sequences for quaternary submixtures

1	A/BCD→B/CD→C/D	1	B/CDE→C/DE→D/E
2	A/BCD→BC/D→B/C	2	B/CDE→CD/E→C/D
3	A/BCD→BC̲D→B/C→C/D	3	B/CDE→CD̲E→C/D→D/E
4	AB/CD→A/B→C/D	4	BC/DE→B/C→D/E
5	ABC/D→AB/C→A/B	5	BCD/E→BC/D→B/C
6	ABC/D→A/BC→B/C	6	BCD/E→B/CD→C/D
7	ABC/D→AB̲C→A/B→B/C	7	BCD/E→BC̲D→B/C→C/D
8	AB̲CD→B/CD→A/B→C/D	8	BC̲DE→C/DE→B/C→D/E
9	AB̲CD→BC/D→A/B→B/C	9	BC̲DE→CD/E→B/C→C/D
10	AB̲CD→BC̲D→A/B→B/C→C/D	10	BC̲DE→CD̲E→B/C→C/D→D/E
11	ABC̲D→A/BC→B/C→C/D	11	BCD̲E→B/CD→C/D→D/E
12	ABC̲D→AB/C→A/B→C/D	12	BCD̲E→BC/D→B/C→D/E
13	ABC̲D→AB̲C→A/B→B/C→C/D	13	BCD̲E→BC̲D→B/C→C/D→D/E
14	AB̲C̲D→A/BC→BC̲D→B/C→C/D	14	BC̲D̲E→B/CD→CD̲E→C/D→D/E
15	AB̲C̲D→A/BC→BC/D→B/C	15	BC̲D̲E→B/CD→CD/E→C/D
16	AB̲C̲D→AB/C→B/CD→A/B→C/D	16	BC̲D̲E→BC/D→C/DE→B/C→D/E
17	AB̲C̲D→AB̲C→BC/D→A/B→B/C	17	BC̲D̲E→BC̲D→CD/E→B/C→C/D
18	AB̲C̲D→AB̲C→BC̲D→A/B→B/C→C/D	18	BC̲D̲E→BC̲D→CD̲E→B/C→C/D→D/E
19	AB̲C̲D→A/BC→B/CD→B/C→C/D	19	BC̲D̲E→B/CD→C/DE→C/D→D/E
20	AB̲C̲D→AB̲C→B/CD→A/B→B/C→C/D	20	BC̲D̲E→BC̲D→C/DE→B/C→C/D→D/E
21	AB̲C̲D→AB/C→BC/D→A/B→B/C	21	BC̲D̲E→BC/D→CD/E→B/C→C/D
22	AB̲C̲D→AB/C→BC̲D→A/B→B/C→C/D	22	BC̲D̲E→BC/D→CD̲E→B/C→C/D→D/E

The following procedure is formulated in which each step is used to determine the distinct separation sequences for one of the first splits of the feed mixture in Table 1.

Step 1. The number of the distinct separation sequences from the first split A/BCDE is 22. This is determined by the heavy subgroup BCDE which can produce 22 distinct sequences as shown in Table 3.

Step 2. The number of the distinct separation sequences from the first split AB/CDE is 3. Since the light subgroup is a binary submixture AB which has the only split A/B, the heavy subgroup CDE determines that there can produce three distinct sequences as shown in Table 2.

Step 3. The number of the distinct separation sequences from the first split ABC/DE is 3 that is determined by the light subgroup ABC which can produce 3 distinct sequences as shown in Table 2.

Step 4. The number of the distinct separation sequences from the first split ABCD/E is 22 that is determined by the light subgroup ABCD which can produce 22 distinct sequences as shown in Table 3.

Step 5. The number of the distinct separation sequences from the first split A$\underline{B}$CDE is 22 that is determined by the heavy subgroup BCDE which can produce 22 distinct sequences as shown in Table 3.

Step 6. The number of the distinct separation sequences from the first split AB$\underline{C}$DE is 9. That is determined by both the light subgroup ABC and the heavy subgroup CDE, each can produce 3 distinct sequences as shown in Table 2.

Step 7. The number of the distinct separation sequences from the first split ABC$\underline{D}$E is 22 that is determined by the light subgroup ABCD which can produce 22 distinct sequences as shown in Table 3.

Step 8. The number of the distinct separation sequences from the first split A$\underline{BC}$DE is 66. That is determined by both the light subgroup ABC and the heavy subgroup BCDE. The light subgroup ABC can produce 3 distinct sequences as shown in Table 2, and the heavy subgroup BCDE can produce 22 distinct sequences as shown in Table 3.

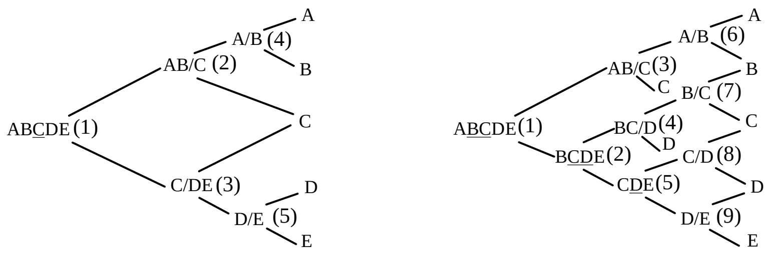
Step 9. The number of the distinct separation sequences from the first split AB$\underline{CD}$E is 66. That is determined by both the light subgroup ABCD and the heavy subgroup CDE. The light subgroup ABCD can produce 22 distinct sequences as shown in Table 3, and the heavy subgroup CDE can produce 3 distinct sequences as shown in Table 2.

Step 10. The number of the distinct separation sequences from the first split A$\underline{BCD}$E is 334. That is determined by both the light subgroup ABCD and the heavy subgroup BCDE. It is noted that the light subgroup ABCD and the heavy subgroup BCDE can simultaneously produce the same submixture BCD in some of the distinct sequences in Table 3. As indicated above, this same submixture simultaneously produced from the two different subgroups must designate one same intended individual split in formulating a feasible separation sequence. From Table 3, it is seen that there are 7 distinct sequences from the light subgroup ABCD (4-7, 11-13 in Table 3) that do not produce the submixture BCD. Each of these 7 distinct sequences can produce 22 functionally distinct sequences for the feed mixture through combination with each of the 22 distinct sequences of the heavy subgroup BCDE as in Table 3. The remaining 15 distinct sequences of the light subgroup ABCD produce the submixture BCD. Simultaneously, there are 7 distinct sequences from the heavy subgroup BCDE (1-4, 8-10 in Table 3) that do not produce the submixture BCD, the remaining 15 distinct sequences of the heavy subgroup BCDE produce the submixture BCD. Obviously, each of the 15 distinct sequences of the light subgroup ABCD with the submixture BCD can combine with each of the 7 distinct sequences of the heavy subgroup BCDE without the submixture BCD. For each of the 15 distinct sequences of the light subgroup ABCD with the submixture BCD, there can identify 5 distinct sequences among the 15 distinct sequences of the heavy subgroup BCDE with the submixture BCD that have the same intended individual split for the submixture BCD. Therefore, each of the 15 distinct sequences of the light subgroup ABCD with the submixture BCD can only combine with 12 of the 22 distinct sequences of the heavy subgroup BCDE. In total, 334 distinct separation sequences are produced from the first split of ABCDE.

Finally, in total, 569 functionally distinct separation sequences are produced from all of the ten first splits for the five-component separations as illustrated in Table 1.

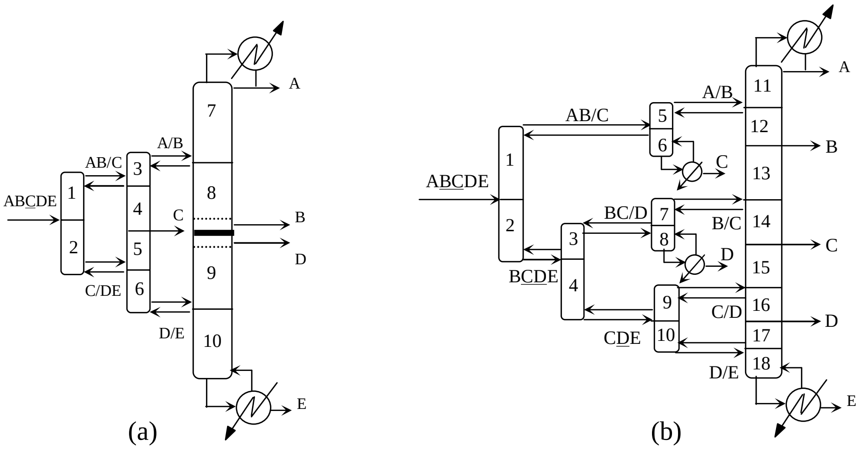
3. Functionally Distinct New Distillation Systems for Five-Component Separations

It is obvious that the functionally distinct separation sequences will designate the functionally distinct distillation systems for the separation task. In order to find the feasible distillation configurations from the identified functionally distinct separation sequences, we need to identify the possible combinations of the intended individual splits in a separation sequence. This can be done by using network structures to represent the distinct separation sequences. Network representations of multicomponent distillation configurations have been presented by Hu et al.(1991) and Agrawal (1996). In an earlier work, it was shown that a network representation of a feasible separation sequence uniquely designates a functionally distinct distillation configuration for a multicomponent distillation (Rong et al., 2003b). For an n-component distillation, there need n layers in the network representation of a distinct separation sequence. The feed is put in the first layer and the products are put in the last layer. The intended individual splits for the submixtures with the same number of components are ranked and put into the same layer in the network representation of a distinct separation sequence (note that some layer(s) could have no splits). Then, the possible combinations of the intended individual splits in the separation sequence at different layers can be determined in the network representation. This will finally determine the interconnections of the column units in the distillation configurations. Because of the space limit, it is impossible to present all of the network structures for all of the distinct separation sequences. As examples, Figure 1 presents two network structures for the following two distinct sequences. Figure 1a is a distinct sequence from the sixth first split: ABCDE(1)→AB/C(2)→C/DE(3)→A/B(4)→D/E(5), Figure 1b is a distinct sequence from the eighth first split: ABCDE(1)→BCDE(2) → AB/C(3) → BC/D(4) → CDE(5) →A/B(6)→B/C(7)→C/D(8)→D/E(9) (number is the order of the intended individual splits). Two feasible distillation configurations of the network structures in Figure 1 are shown in Figure 2.



(a) (b)

Figure 1. Network structures of two distinct sequences for a five-component mixture



(a) (b)

Figure 2. New Distillation configurations from the distinct sequences in Figure 1

It should be noted that some distinct sequences produce only one network structure, while others can produce several different network structures. For example, the distinct sequence in Figure 1b can produce four different network structures through different combinations of the middle component products C and D between the intended individual splits (1. (7)+(8)→C, (8)+(9)→D; 2. (3)+(8)→C, (8)+(9)→D; 3. (7)+(8)→C, (4)+(9)→D; 4. (3)+(8)→C, (4)+(9)→D). Each network structure can produce a feasible distillation configuration for the separation task (Rong et al. 2003b).

4. Conclusions

Systematic synthesis of all of the distillation configurations for five-component separations has been presented in this work. The first splits of the feed mixture have been used to generate the distinct separation sequences. The distinct sequences for each of the first splits for a five-component separation have been identified based on the distinct sequences for ternary and quaternary submixtures. The feasible distillation configurations have been obtained by network structures of the intended individual splits in the distinct sequences. They include the traditional distillation configurations, the distinct thermally coupled configurations, from which the other possible distillation configurations can be produced. This formulates a complete space of possible alternatives for five-component distillations to look for an optimal system for a specific application.

References

Agrawal R., 1996, Ind. Eng. Chem. Res., 35, 1059.
Agrawal R., 2003, AIChE J., 49, 379.
Heaven D. L., 1969, M.S. Thesis, University of California, Berkeley, CA.
Hu Z., Chen B., Rippin D.W.T.,1991, AIChE Annual Meeting,Los Angeles,Paper 155b.
Kaibel G., Schoenmakers, H., 2002, Computer-Aided Chem. Eng. 14, ESCAPE 12, p.9.
Rathore R.N.S., Wormer K.A.V., Powers G.J., 1974, AIChE J., 20, 940.
Rong B.-G., Kraslawski A., Turunen I., 2003a, Ind. Eng. Chem. Res., 42, 4329.
Rong B.-G., Kraslawski A., Turunen I., 2003b, Ind. Eng. Chem. Res., 42, 1204.