

# Partially Thermally Coupled Distillation Systems for Multicomponent Separations

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Distillation is the largest energy consumer among process units. A large amount of research work has been done toward improving the energy efficiency of distillation systems either in terms of the design of optimal distillation schemes or improving internal column efficiency. Still, the optimal design and synthesis of multicomponent distillation systems is one of the most challenging problems in process engineering.

For multicomponent distillations, the thermal-coupling technique can be used to design distillation systems that have the potential to reduce significantly both energy consumption and capital cost in comparison to the conventional simple column configurations. Since the invention of the thermally coupled distillation column by Wright (1949), numerous studies have been conducted. However, due to the complexity, research on these new configurations is mostly restricted to ternary mixtures. The most commonly studied thermally coupled schemes are the side-stripper (SS), the side-rectifier (SR), and the fully coupled scheme (FC) (the so-called Petlyuk column) (Petlyuk et al., 1965).

A few interesting observations have been obtained for ternary thermally coupled schemes. For example, the FC configuration has been proved to have the minimum total vapor flow compared with other thermally coupled schemes (Fidkowski and Krolkowski, 1987). Among the three thermally coupled schemes, over a wide range of relative volatilities and feed compositions, the SR and the SS configurations can have a similar heat demand than the FC configuration (Agrawal and Fidkowski, 1999). It is also recognized that the thermodynamic efficiency of a fully thermally coupled configuration can often be inferior because all of its heat is received at the highest temperature and rejected at the lowest temperature (Carlberg and Westerberg, 1989). Thanks to the intensive research work on the thermally coupled schemes for ternary mixtures, the FC system has been successfully used in many industrial cases in its dividing-wall arrangement (Becker et al., 2001).

As for thermally coupled schemes for mixtures with four or more components, there are only a few reports in the litera-

ture. These are mostly concerned with finding the possible structures of the thermally coupled schemes. Sargent and Gaminibandara (1976) presented a superstructure for a four-component, fully coupled scheme. Kaibel (1987) and Christiansen et al. (1997) illustrated some distillation columns with vertical partitions for multicomponent separations. From a simple column configuration (SC), Agrawal (1996) presented some observations to generate the special fully coupled schemes with satellite column arrangements for four or more component mixtures. From a known FC configuration of a multicomponent distillation, Agrawal (2000) has illustrated how to draw its thermodynamic equivalent structures. It is interesting to note that the available works on thermally coupled schemes for mixtures with four or more components are mainly concerned with the FC schemes. However, it must be recognized that there are two different subspaces among all of the possible thermally coupled schemes for mixtures with four or more components. One is constituted by the partially thermally coupled schemes (PC) with only sharp splits, and the other is composed of the FC schemes that include sloppy split(s). A very brief analysis shows that the PC distillation schemes are characterized by the minimum number of column sections and a lower number of condenser(s) and/or reboiler(s) than the SC configurations, as well as fewer inter-column communicating streams than the FC schemes. These features make them very attractive in view of energy conservation due to the thermal couplings, and savings of capital cost due to the reduced number of heat exchangers and minimum number of column sections. It also has better controllability and operability with the minimum number of intercolumn communicating streams compared with the FC schemes.

As will be illustrated in the next section, the subspace of the PC schemes can be exactly mapped from the subspace of the SC configurations for any  $n$ -component mixtures. There are well-known works on the systematic synthesis of optimal SC systems in the complete subspace of the SC configurations for four or more component mixtures (Thompson and King 1972; Rathore et al., 1974); however, there is no study on the systematic synthesis of the optimal PC schemes in the complete subspace of these schemes for four or more compo-

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nent mixtures. A lack of knowledge and design tools is the main barrier for the utilization of these simple multicomponent thermally coupled schemes in process industries.

The main purpose of this article is to systematically synthesize the complete subspace of the PC distillation systems for any  $n$ -component mixtures, with a focus on a detailed parametric comparison of the PC systems with those SC configurations for a five-component mixture. These comparisons are aimed at obtaining insights about the PC systems for multicomponent distillations.

## Partially Thermally Coupled Distillation Systems for Four or More Component Mixtures

In this article, our definition of PC distillation systems for multicomponent separations is that they have the same individual sharp splits as conventional simple column configurations, while the column units are interconnected by the thermal coupling streams. These partially coupled systems can be exactly mapped from the SC configurations for any  $n$ -component mixture ( $n \geq 3$ ). In a conventional SC configuration for an  $n$ -component distillation, there are a total of  $n-1$  simple columns (Petlyuk et al. 1965; Thompson and King, 1972), each one has a rectifying column section with a condenser and a stripping section with a reboiler. In consequence, each SC configuration has in all  $2(n-1)$  column sections, as well as  $2(n-1)$  condensers and reboilers. It is observed that among  $2(n-1)$  column sections in an SC configuration, there are  $n$  column sections that produce the desired pure products from the corresponding condenser(s) and reboiler(s). Each of these  $n$  column sections is enriched with one of the components in the feed mixture. While the remaining  $n-2$  column sections do not produce the desired pure products, their condenser(s) and/or reboiler(s) have submixtures with two or more components. Thus, each of these  $n-2$  column sections is enriched with a submixture containing two or more components. One can expect that even if the column section does not produce the desired pure product, it still functions as a separation unit with multiple equilibrium stages (or a certain height of packings) in which the submixture is prefractionated to a certain extent. However, the prefractionation is disturbed in conventional SC configurations due to the remixing in the condenser or the reboiler at the end of the column section. According to Petlyuk et al. (1965), this remixing can be avoided by removing the condenser or the reboiler at the end of the column section and interconnecting the column units by a two-way liquid and vapor streams, that is, the thermal coupling streams. After its condenser (reboiler) is removed, each rectifying (stripping) column section will require liquid reflux (vapor boilup) from its subsequent column unit. In this way, it is expected that the prefractionation realized in the column section of the previous column unit can be inherited in the subsequent column unit, thus reducing the irreversibility of the separation process and improving the separation efficiency. Triantafyllou and Smith (1992) and Finn (1993) have clearly demonstrated the prefractionation and the remixing phenomena in their case studies.

The PC system for an  $n$ -component distillation is made by removing all of the  $n-2$  condenser(s) and/or reboiler(s) associated with those  $n-2$  column sections that lack the pure products of the conventional SC configuration, and introduc-

**Table 1. Simple Column Sequences for a Five-Component Mixture**

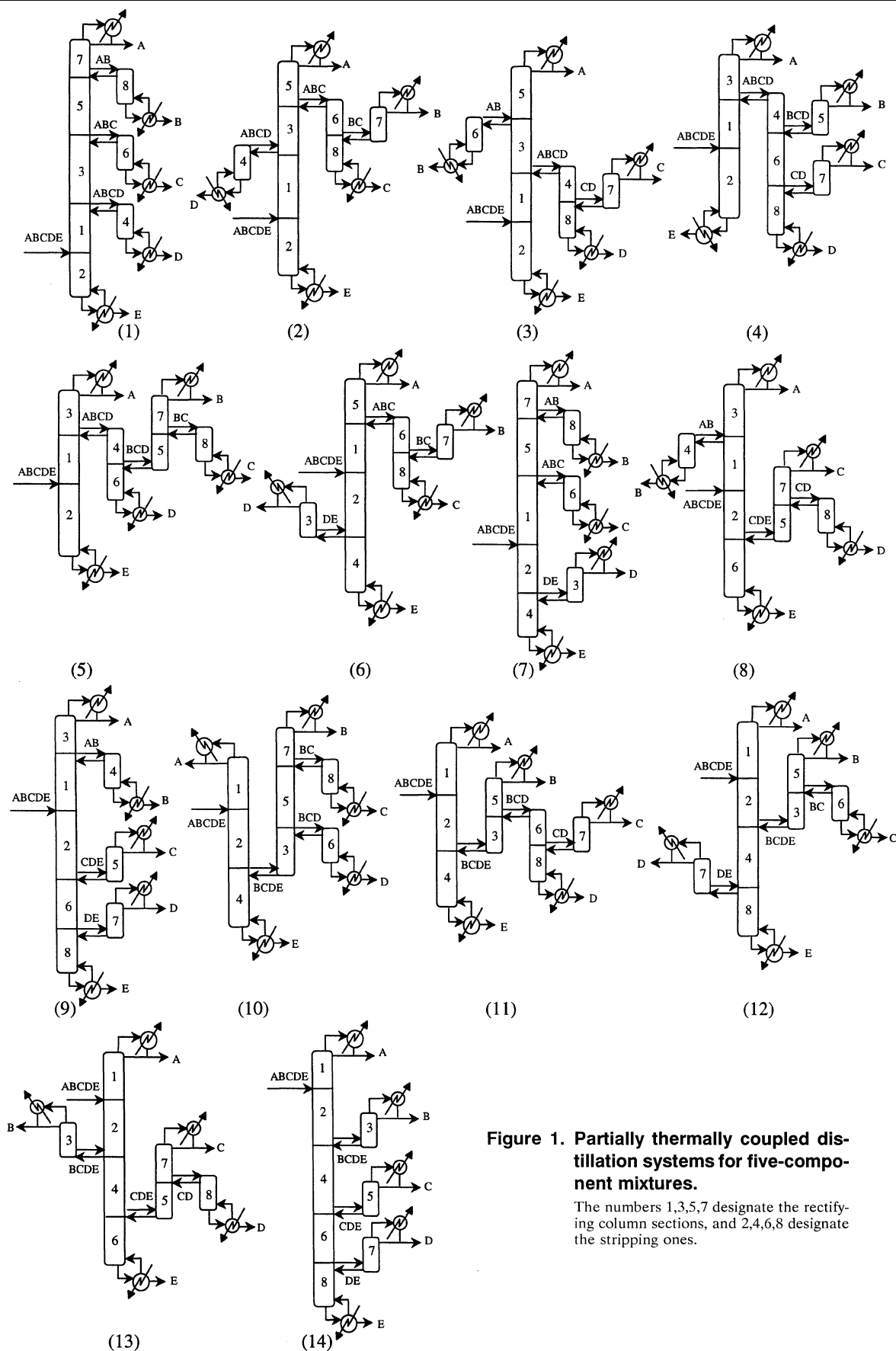
| Sequence No. | Simple Column Sequences     |
|--------------|-----------------------------|
| 1            | ABCD/E → ABC/D → AB/C → A/B |
| 2            | ABCD/E → ABC/D → A/BC → B/C |
| 3            | ABCD/E → AB/CD → A/B → C/D  |
| 4            | ABCD/E → A/BCD → B/CD → C/D |
| 5            | ABCD/E → 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 |

ing  $n-2$  two-way thermal coupling streams into the system. Thus, the total number of PC systems ( $S_n$ ) for any  $n$ -component distillation is equal to the total number of conventional SC configurations for any  $n$ -component distillation that can be calculated by the following equation of Thompson and King (1972)

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

Obviously, the PC distillation systems constitute a complete subspace for any  $n$ -component mixture that can be exactly mapped from the subspace of the conventional SC configurations. For example, the subspace of the 14 simple column sequences for a five-component mixture is presented in Table 1. The subspace of the corresponding 14 partially thermally coupled systems is illustrated in Figure 1.

Briefly, generation of the subspace of the partially coupled schemes for any  $n$ -component mixture can be completed by the following steps: (1) generate the subspace of the SC configurations (for example, Thompson and King, 1972); (2) identify the  $n-2$  condenser(s) and/or reboiler(s) with submixtures of two or more components for each of the SC configurations; (3) remove those identified condenser(s) and/or reboiler(s) with submixtures of two or more components and introduce two-way thermal coupling streams for each condenser and reboiler removed; (4) combine the stripping column sections receiving the vapor flows from the same reboiler and the rectifying column sections receiving the liquid flows from the same condenser. Following this procedure, the partially coupled system obtained has a main column that produces the products of the most volatile component from the top condenser and the least volatile component from the bottom reboiler. The other  $n-2$  column units are SSs and/or SRs with the products of intermediate components, like the subspace of the partially coupled systems in Figure 1 for five-component mixtures. It should be indicated that, apart from these PC systems, the other possible thermally coupled schemes can also be produced for four or more component mixtures, for instance, the thermally coupled schemes with a lower number of thermal couplings than PC systems, as well as the thermally coupled schemes with fewer heat exchangers



**Figure 1. Partially thermally coupled distillation systems for five-component mixtures.**

The numbers 1,3,5,7 designate the rectifying column sections, and 2,4,6,8 designate the stripping ones.

**Table 2. Feed Components and Mole Fractions**

| Component            | Mole Fraction | $T_b$ (K) | $\Delta T_b$ (K) |
|----------------------|---------------|-----------|------------------|
| A Ethanol            | 0.25          | 351.5     | —                |
| B Isopropanol        | 0.15          | 355.4     | 3.9              |
| C <i>n</i> -Propanol | 0.35          | 370.4     | 15.0             |
| D Isobutanol         | 0.10          | 381.0     | 10.6             |
| E <i>n</i> -Butanol  | 0.15          | 390.9     | 9.9              |

than PC systems. The relative advantages of these different thermally coupled schemes for four or more component mixtures will be case-based in terms of energy savings, capital cost, as well as operability. The PC systems generated have formulated a unique subspace among all of the possible thermally coupled schemes for four or more component mixtures.

The distinct features of the PC systems are as follows: (1) they have the same  $n-1$  individual sharp splits as the conventional SC configurations; (2) they have the same minimum number of  $2(n-1)$  column sections as the conventional SC configurations; (3) they have less  $n-2$  heat exchangers than the conventional SC configurations; (4) they have  $n-2$  introduced thermal coupling streams. These features make the systems relatively uncomplicated, and in consequence they are more amenable to control and operation. At the same time, they have the potential to significantly reduce both the energy consumption and capital costs. Furthermore, a noteworthy structural feature of a partially coupled system is that there is flexibility in determining the arrangement of its column sections. For a partially coupled scheme, this can produce so-called thermodynamic equivalent structures through rearrangements of the column sections. This flexibility in structural arrangement gives us the freedom to design thermally coupled systems with specific concerns, for instance, column equipment designs. It might also affect the capital cost of a partially coupled system through different arrangements of the column sections.

In the next section we will show that in the systematic synthesis of the optimal PC system in the complete PC subspace, the dominant evaluation metric to distinguish all of the PC systems is the operating cost that corresponds to the total vapor flow rate. Since all the thermodynamic equivalent structures of a PC system have essentially the same nominal total vapor flow rate, even though there are differences in capital costs among the thermodynamic equivalent structures, these differences will unlikely change the relative advantages of all of the PC systems with SSs and/or SRs, like the structures in Figure 1, evaluated based on the total annual costs. It is interesting to note that this observation for PC systems is the same as for the *heuristic* for the synthesis of

the optimal conventional SC configurations, that is, the total vapor boilup correlates reasonably well with the total annual cost of the simple column sequences (Malone et al., 1985).

### A Case Study for Synthesis of the Partially Coupled Distillation Systems for a Five-Component Mixture

In a multicomponent PC system, the introduction of each thermal coupling is aimed at avoiding the remixing of the prefractionation of a submixture with two or more components in a certain column section of the conventional SC configuration. As a consequence, the separation efficiency of the PC system is expected to be improved compared with its SC counterpart. This, together with the reduction in the number of the heat exchangers, will provide the potential to reduce both the energy consumption and the capital costs in a PC system. Although much work has been conducted on the synthesis of the conventional SC configurations for mixtures with four or more components, work on the systematic synthesis of the PC systems for mixtures with four or more components is still lacking in the open literature. In this section, we present a systematic synthesis of the PC systems for the separation of a five-component mixture. Both the subspace of the 14 SC configurations and the subspace of the 14 PC systems are included in the synthesis space. The synthesis is based on comparisons of the operating and capital costs of the PC systems with the SC configurations. To calculate the operating and the capital costs for the PC systems, a design procedure has been developed for designing the partially coupled configurations for multicomponent separations (Rong et al., 2001). The capital cost is estimated based on the correlations and data in Douglas (1988). It must be pointed out that the procedure for calculating the capital cost of a distillation column presented in Appendix A of Douglas' book (1988) is determined for a single column. The capital cost of a column is estimated based on the calculations of the diameter and the height for the column. However, in a multicomponent distillation configuration, there are several columns, and the calculations of the heights for the different columns can follow different constraints. This may result in estimations of the capital costs of the columns based on the different metrics in different configurations. In this work, it is observed that, to calculate the capital cost of a column unit in a multicomponent distillation scheme, it is more rational to use the number of theoretical plates as the column height.

The five-component separation problem is presented in Table 2 (Andreovich and Westerberg, 1985), where  $T_b$  is the normal boiling point (K) and  $\Delta T_b$  is the difference of the normal boiling points of the adjacent components. The feed flow rate is 500.4 kmol/h and the recovery for the key components in each column is 0.98. Table 3 contains information about the utilities for calculating the operating costs (Douglas, 1988).

The calculated results of the total vapor rate, the capital cost of the heat exchangers, and the capital cost of the columns for each of the 14 SC configurations and each of the 14 PC systems are presented in Tables 4 and 5, respectively. The heat demands and the annualized capital and operating costs, as well as the total annual cost for each of the 14 SC configurations and each of the 14 PC systems are shown in

**Table 3. Available Utilities for Systems Synthesis**

| Utilities          | Temp. (K) | Cost (US\$/1,000 kg) |
|--------------------|-----------|----------------------|
| Cooling water      | 305.15    | 0.1323               |
| Steam (0.1034 MPa) | 373.15    | 5.0274               |
| Steam (0.3447 MPa) | 410.15    | 6.1740               |
| Steam (1.0342 MPa) | 453.15    | 7.4970               |
| Steam (1.7237 MPa) | 480.15    | 8.2026               |
| Steam (4.1369 MPa) | 523.15    | 9.9666               |

**Table 4. Total Vapor Flow Rate and Equipment Data of Simple Column Configurations in Table 1**

| Seq. No. | Total Vapor Flow Rate (kmol/h) | Total No. of Theor. Plates | Total Area of Heat Exchangers (m <sup>2</sup> ) | Total Cost of Heat Exchangers (10 <sup>4</sup> US\$) | Total Cost of Towers (10 <sup>4</sup> US\$) |
|----------|--------------------------------|----------------------------|---|--|---|
| 1        | 4,403.4                        | 233                        | 3,000.0   | 310.6  | 534.2                                       |
| 2        | 4,668.9                        | 256                        | 3,186.3   | 316.3  | 654.6                                       |
| 3        | 4,122.8                        | 231                        | 2,773.1   | 293.7  | 550.7                                       |
| 4        | 4,336.1                        | 249                        | 2,923.4   | 298.0  | 624.4                                       |
| 5        | 4,403.0                        | 249                        | 2,983.0   | 302.4  | 636.8                                       |
| 6        | 4198.6                         | 256                        | 2,844.4   | 287.2  | 625.6                                       |
| 7        | 3,933.4                        | 232                        | 2,658.4   | 281.4  | 505.1                                       |
| 8        | 3,910.1                        | 231                        | 2,597.3   | 280.1  | 535.5                                       |
| 9        | 3,692.3                        | 231                        | 2,456.5   | 266.9  | 521.7                                       |
| 10       | 4,267.2                        | 248                        | 2,877.8   | 294.1  | 635.5                                       |
| 11       | 4,200.5                        | 249                        | 2,818.3   | 289.8  | 623.2                                       |
| 12       | 3,945.8                        | 248                        | 2,657.0   | 274.3  | 606.2                                       |
| 13       | 4,140.0                        | 248                        | 2,767.0   | 285.9  | 607.8                                       |
| 14       | 3,922.5                        | 249                        | 2,626.6   | 272.7  | 594.1                                       |

Tables 6 and 7, respectively. A capital charge factor of 0.1 is used to annualize the installed cost of the equipment, and the plant operating time is set to be 8,000 h per annum (p.a.). The configurations in both Tables 6 and 7 are ranked based on the increase in their total annual costs.

Based on the calculated results presented in Tables 4 and 5, we have observed that:

1. The total vapor flow rates of the PC systems are much lower than their SC counterparts. The maximum saving in the total vapor flow rate corresponds with separation se-

**Table 5. Total Vapor Flow Rate and Equipment Data of the Partially Coupled Systems in Figure 1**

| Scheme No. | Total Vapor Flow Rate (kmol/h) | Total No. of Theor. Plates | Total Area of Heat Exchangers (m <sup>2</sup> ) | Total Cost of Heat Exchangers (10 <sup>4</sup> US\$) | Total Cost of Towers (10 <sup>4</sup> US\$) |
|------------|--------------------------------|----------------------------|---|--|---|
| 1          | 3,399.5                        | 234                        | 2,396.3   | 212.2  | 634.8                                       |
| 2          | 3,508.2                        | 264                        | 2,450.2   | 210.8  | 760.6                                       |
| 3          | 3,570.7                        | 234                        | 2,407.7   | 220.2  | 581.9                                       |
| 4          | 3,624.8                        | 258                        | 2,406.7   | 210.3  | 774.4                                       |
| 5          | 4,054.1                        | 253                        | 2,705.2   | 237.4  | 758.1                                       |
| 6          | 3,407.3                        | 266                        | 2,332.6   | 201.7  | 734.4                                       |
| 7          | 3,217.1                        | 237                        | 2,219.7   | 199.7  | 611.5                                       |
| 8          | 3,276.3                        | 234                        | 2,159.0   | 207.9  | 583.1                                       |
| 9          | 3,109.3                        | 239                        | 2,034.8   | 193.2  | 559.0                                       |
| 10         | 3,847.2                        | 253                        | 2,554.8   | 228.6  | 764.5                                       |
| 11         | 4,057.5                        | 256                        | 2,598.9   | 234.7  | 727.4                                       |
| 12         | 3,563.1                        | 259                        | 2,325.1   | 206.6  | 716.5                                       |
| 13         | 3,372.5                        | 261                        | 2,172.9   | 197.7  | 730.1                                       |
| 14         | 3,127.1                        | 266                        | 2,020.3   | 178.8  | 734.1                                       |

**Table 6. Synthesis Results of the Simple Column Configurations in Table 1**

| Seq. No. | Total Heat of Reboilers (10 <sup>6</sup> kJ/h) | Total Heat of Condensers (10 <sup>6</sup> kJ/h) | Capital Cost (10 <sup>4</sup> US\$/yr) | Operating Cost (10 <sup>4</sup> US\$/yr) | Total Cost (10 <sup>4</sup> US\$/yr) |
|----------|--|---|--|--|--------------------------------------|
| 9        | 142.4  | 145.3   | 78.9                                   | 405.3                                    | 484.2                                |
| 8        | 150.7  | 154.1   | 81.6                                   | 412.4                                    | 494.0                                |
| 7        | 151.6  | 154.5   | 78.7                                   | 437.5                                    | 516.2                                |
| 14       | 153.7  | 154.1   | 86.7                                   | 434.1                                    | 520.8                                |
| 3        | 158.7  | 162.4   | 84.4                                   | 440.1                                    | 524.5                                |
| 12       | 154.5  | 154.9   | 88.1                                   | 438.8                                    | 526.9                                |
| 13       | 162.0  | 162.9   | 89.4                                   | 441.1                                    | 530.5                                |
| 11       | 164.1  | 165.4   | 91.3                                   | 449.4                                    | 540.7                                |
| 10       | 166.6  | 167.9   | 93.0                                   | 456.1                                    | 549.1                                |
| 1        | 169.6  | 173.3   | 84.5                                   | 468.5                                    | 553.0                                |
| 4        | 168.3  | 170.8   | 92.2                                   | 464.6                                    | 556.8                                |
| 6        | 162.9  | 165.0   | 91.3                                   | 466.3                                    | 557.6                                |
| 5        | 170.8  | 173.3   | 93.9                                   | 471.3                                    | 565.2                                |
| 2        | 180.9  | 183.8   | 97.1                                   | 497.4                                    | 594.5                                |

**Table 7. Synthesis Results of the Partially Thermally Coupled Systems in Figure 1**

| Scheme No. | Total Heat of Reboilers (10 <sup>6</sup> kJ/h) | Total Heat of Condensers (10 <sup>6</sup> kJ/h) | Capital Cost (10 <sup>4</sup> US\$/yr) | Operating Cost (10 <sup>4</sup> US\$/yr) | Total Cost (10 <sup>4</sup> US\$/yr) |
|------------|--|---|--|--|--------------------------------------|
| 9          | 118.1  | 121.4   | 75.2                                   | 352.6                                    | 427.8                                |
| 7          | 122.3  | 125.6   | 81.1                                   | 355.1                                    | 436.2                                |
| 8          | 124.8  | 128.5   | 79.1                                   | 374.9                                    | 454.0                                |
| 1          | 129.0  | 132.7   | 84.7                                   | 375.8                                    | 460.5                                |
| 14         | 118.9  | 121.0   | 91.3                                   | 390.4                                    | 481.7                                |
| 3          | 135.7  | 139.4   | 80.2                                   | 412.5                                    | 492.7                                |
| 13         | 129.0  | 131.0   | 92.8                                   | 423.1                                    | 515.9                                |
| 6          | 130.2  | 132.7   | 93.6                                   | 427.6                                    | 521.2                                |
| 12         | 136.5  | 136.9   | 92.3                                   | 434.6                                    | 526.9                                |
| 2          | 134.0  | 136.9   | 97.1                                   | 439.3                                    | 536.4                                |
| 4          | 136.9  | 140.7   | 98.5                                   | 450.5                                    | 549.0                                |
| 10         | 148.2  | 148.2   | 99.3                                   | 471.6                                    | 570.9                                |
| 5          | 154.1  | 156.6   | 99.5                                   | 493.5                                    | 593.0                                |
| 11         | 155.3  | 156.6   | 96.2                                   | 509.8                                    | 606.0                                |

quence 2. It is 25% lower for the PC system than its SC counterpart. The average saving in the total vapor flow rates of the PC systems is 15.5%, as compared to the SC configurations.

2. The PC systems have a slightly higher total number of theoretical plates than their SC counterparts. This is because the designed operating pressures of the PC systems are a little higher than their SC counterparts, and this increase in pressure is due to the constraints of the vapor flows of the thermal coupling streams on the PC systems. Thus, the relative volatilities of the components in the PC systems are a little lower than in the SC configurations. This results in an increase in the number of theoretical plates for the PC systems. Moreover, it reduces the potential reduction in the number of theoretical plates for the PC systems by the inheritance of the prefractionations of the submixtures in certain column sections of the corresponding SC configurations.

3. The total area of condensers and reboilers in the PC system is much smaller than in its SC counterpart. The average reduction in the total area of the heat exchangers of the PC systems is about 16.3% in comparison to the SC configurations. The maximum reduction is about 23.1%, which corresponds to configurations 2 and 14 in Figure 1. Therefore, it contributes to a big savings in the total cost of the condensers and reboilers in the PC systems. The average savings in the total cost of the heat exchangers in the PC systems is about 27.5% in comparison to the SC configurations, and the maximum saving is 34.4% compared to sequence 14.

4. The total cost of the towers presented in Table 5 for the PC systems is much higher than for the SC configurations in Table 4. This is somehow counterintuitive, because there is a significant reduction in the total vapor flow rate in the PC system and the number of the total theoretical plates for the PC system is almost the same as its SC counterpart. The main reason for such a situation is that for the SC configurations with saturated liquid feeds, the diameter of each single column is exactly calculated based on the vapor flow rate in the column, while for the PC systems, the column unit(s) that are connected by the thermal coupling streams with other column unit(s) have different vapor flow rates in different column sections. In this situation, the maximum vapor flow rate is determined by calculating the column diameter. This is the

**Table 8. Synthesis Results Based on the Revised Tower Cost Estimations for PC Systems in Figure 1**

| Scheme No. | Total Cost of Towers (10 <sup>4</sup> US\$) | Annualized Capital Cost (10 <sup>4</sup> US\$/yr) | Total Cost (10 <sup>4</sup> US\$/yr) |
|------------|---|---|--------------------------------------|
| 9          | 454.5                                       | 64.8  | 417.4                                |
| 7          | 422.0                                       | 62.3  | 417.4                                |
| 1          | 414.2                                       | 62.6  | 438.4                                |
| 8          | 454.5                                       | 66.2  | 441.1                                |
| 14         | 506.0                                       | 68.5  | 458.9                                |
| 3          | 483.1                                       | 70.3  | 482.8                                |
| 13         | 521.1                                       | 71.9  | 495.0                                |
| 6          | 527.5                                       | 72.9  | 500.5                                |
| 2          | 507.2                                       | 71.8  | 511.1                                |
| 12         | 571.7                                       | 77.8  | 512.4                                |
| 4          | 540.8                                       | 75.1  | 525.6                                |
| 10         | 584.5                                       | 81.3  | 552.9                                |
| 5          | 595.7                                       | 83.3  | 576.8                                |
| 11         | 618.9                                       | 85.4  | 595.2                                |

most conservative way to calculate the costs of the towers in the PC systems. The synthesis results of the PC systems presented in Table 7 are based on this conservative estimation of the total cost of the towers for the PC systems. An alternative way of estimating the total cost of the towers for the PC systems is based on the total vapor flow rate and the total number of theoretical plates. The results obtained, together with the synthesis results for the PC systems, are presented in Table 8. It can be seen that the total cost of the towers of the PC system in Table 8 is much lower than for its SC counterpart in Table 4. The average saving is about 13%, and the maximum saving is about 22.5%, which corresponds to sequences 1 and 2.

From the synthesis results presented in Tables 6, 7, and 8, we have observed that:

1. The heat demand for each PC system is much lower than its SC counterpart. The average saving is about 16.8%, and the maximum saving is about 26% for sequence 2. The total heat duty of the condensers is approximately equal to the total heat duty of the reboilers in each PC system. It is interesting that this observation is analogous to the remarks by Andreovich and Westerberg (1985) for the SC configurations.

2. The annualized capital cost of each PC system presented in Table 7 is approximately the same as its SC counterpart in Table 6. This means that the cost saving of the heat exchangers in a PC system is counterbalanced by the increase in the cost of the towers based on the maximum vapor flow rates in the columns. The annualized capital costs of the PC systems presented in Table 8, based on the cost of the towers calculated from the total vapor flow rate, are much lower than those of the SC configurations. The average saving is about 18%, and the maximum saving is about 26% for sequences 1 and 2.

3. From Tables 6 and 7, we can see that there are five PC systems (that is, 9, 7, 8, 1, and 14 in Table 7) that are more advantageous than the best SC configuration (sequence 9 in Table 6) with respect to the total annual cost. The best PC system accounts for about a 12% reduction of the total annual cost in comparison to the best SC configuration. Making a one-by-one comparison of the PC system with its SC counterpart in terms of the total annual cost, we can see that there are 11 PC systems (1–4, 6–9, 12–14 in Figure 1) that are more profitable than their SC counterparts. The other three PC systems (5, 10, and 11 in Figure 1) are less profitable than their SC counterparts. Thus, for a specific multicomponent distillation, the synthesis of the optimal PC system must be based on the evaluations from detailed calculations.

4. It is seen from Table 7 that the best PC systems tend to have the big savings on the annual operating costs of their SC counterparts. For example, each of the first five best PC systems (9, 7, 8, 1, and 14 in Figure 1) makes a big saving on the annual operating cost compared to its SC counterpart. The savings on the annual operating costs of PC systems 1, 7, and 9 are 19.8%, 18.8% and 13.0% respectively, in comparison to their SC counterparts, which are the first three biggest savings on their annual operating costs among all the 14 PC systems. The three worst PC systems 10, 5, and 11 are the only ones among all of the PC systems that have higher annual operating costs than their SC counterparts. This shows that the difference in the total annual costs between the best PC system and the worst one is much greater than the difference in the total annual cost between the best SC configuration and the worst one. The difference is about 42% for the PC systems between 9 and 11 in Table 7; in Table 8, the difference is about 43% between PC systems 9 and 11; while for the SC configurations in Table 6, the difference is about 23% between SC configurations 9 and 2.

5. From Tables 6 and 7, we can see that the annual operating cost, compared with the annual capital cost, is the dominant part of the total annual cost for both the SC configurations and the PC systems. For the SC configurations in Table 6, the annual operating cost is, on average, about 83.6% of the total annual cost, while for the PC systems in Table 7, it is, on average, about 82.4%. Thus, the optimal scheme, in either the subspace of the SC configurations in Table 6 or in the subspace of the PC systems in Table 7, is the one with minimum annual operating cost. This is the reason why in Table 8, with the estimated lower cost of the towers for the PC systems, the synthesis results are not much different from the results presented in Table 7 for the synthesis of the PC systems. One can conclude, therefore, that the differences between the capital costs among the thermodynamic-equivalent systems of a PC scheme would not change the synthesis results for the subspace of the PC systems in Figure 1.

6. It is observed, based on the synthesis results in Tables 6, 7, and 8, that the best PC systems for this case are generated from the best SC configurations. Thus, for the synthesis of the PC systems for multicomponent distillations, it is likely that the best PC systems tend to be generated from the best SC configurations. This observation should be confirmed for other cases. If it was confirmed, then the proposed heuristics for the synthesis of the optimal SC configurations from the SC subspace can be used for the synthesis of the optimal PC systems from the PC subspace.

## Conclusions

A complete subspace of the partially thermally coupled (PC) distillation systems has been mapped from the subspace of the conventional simple column (SC) configurations for any  $n$ -component mixture. These PC systems have the same minimum number of  $2(n-1)$  column sections as the SC configurations, while they have less  $n-2$  condenser(s) and/or reboiler(s) than the SC configurations. They have  $n-2$  thermal couplings among the column units, which is the minimum number of thermal couplings compared with the fully thermally coupled schemes. These distinct features make them attractive not only with respect to energy and capital cost savings, but also with regard to operability and controllability. Thus, the PC distillation systems constitute an important subspace for the synthesis of the optimal distillation systems for multicomponent distillations.

A systematic synthesis of the PC systems for a five-component mixture has been performed. Both the subspace of the 14 PC systems and the subspace of the 14 SC configurations are included. The synthesis is based on detailed parametric comparisons of all of the PC systems with all of the SC configurations in terms of both operating and capital costs. The synthesis results clearly demonstrated the advantages of the PC systems over the SC configurations with respect to both energy and capital cost savings. The observations obtained from the synthesis results can help to identify and design the optimal PC system from the overall subspace of the PC systems. We recommend two main steps for the synthesis of an optimal PC system for a specific multicomponent distillation. The first is to look for the best one in the subspace of the PC systems. This can be done either based on the annual operating costs or the total annual costs of the PC systems. The second is to look for the final optimal PC system among the thermodynamic equivalent structures of the best PC system obtained in the first step. This should be based on the total annual costs of the possible thermodynamic equivalents, as well as their operability and controllability.

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