Design and Control Properties of Arrangements for Distillation of Four Component Mixtures Using Less Than N-1 Columns

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The design and study of dynamic properties of distillation sequences using side-stream columns with less than N-1 columns for separation of four-component mixtures were studied. Total annual cost and dynamic properties (using singular value decomposition) were used to compare properties of arrangements with less than N-1 columns to base cases with three columns (conventional case). Quaternary feeds containing four hydrocarbons were analyzed. For systems with low concentrations of one component in the feed, side-stream cascades often show significantly lower operating, capital costs and best dynamic properties compared to the base cases. Low purity requirements also favor side-stream cascades. Some rules are presented to predict which sequence will have the lowest energy consumption capital cost and better dynamic properties.

Key words:
Complex distillation, energy consumption, dynamic properties

Introduction

Most chemical processes are dominated by the need to separate multicomponent chemical mixtures. The dominant choice to carry out such separation tasks is provided by the use of distillation processes. On a global basis, distillation columns consume a large portion of the total industrial heat consumption, so even small improvements which become widely used, can save huge amounts of energy. To improve the energy efficiency of separation processes based on distillation, several strategies have been proposed. The optimal design and synthesis of multicomponent distillation systems remains one of the most challenging problems in process engineering. Many works have been realized on some specific configurations for ternary mixtures, aiming at performance analysis and industrial applications. (Tedder and Rudd;[1] Meszaros and Fonyo;[2] Grossmann *et al.*;[3] Kim;[4] Yeomans and Grossmann;[5] Rong *et al.;*[6] Caballero and Grossmann;[7] Kim *et al.*;[8] Rong and Kraslawski;[9] Kim *et al.*;[10] Barttfeld *et al.*;[11] Rong and Turunen,[12] among others). When the number of products is three or four, designing and costing all possible sequences can best determine the most economical sequence. Often, however, unless the feed mixture has a wide distribution of component concentrations or a wide variation of relative volatilities, it may be based on operation factors. In that case, the direct sequence is often the choice. Otherwise, a number of heuristics and mathematical methods that have appeared in literature have proved useful for reducing the number of sequences for detailed examination (Hendry and Hughes;[13] Thompson and King;[14] Rodrigo and Seader;[15] Gómez and Seader;[16] Seader and Westerberg;[17] Modi and Westerberg[18]). Tedder and Rudd[1] first developed the criteria for use of side streams for the separation of ternary mixtures that do not exhibit azeotropes, and suggested taking a vapor as a side-stream product if the side stream is below the feed, and a liquid product if the side stream is above the feed. Also, they developed heuristics of when a single column can be used for separation of ternary mixtures. Most of the studies have focused on complete separation of *N* component mixtures using N-1 distillation columns with a reboiler at the bottom and a condenser at the top of each column. There are very few works on configurations of four or more component mixtures, especially on the parametric studies of the performance of such multicomponent complex distillation flowsheets by computational work (Agrawal;[19] Christiansen *et al.*[20]). However, cascades that use less than N-1 columns for multicomponent distillation processes have not been extensively studied (for example Rooks *et al.*;[21] Kin and Wankat[22]).

In this paper (an extension of the work of Kin and Wankat[22]) we study the design and control properties of eleven distillation arrangements with less than N-1 columns (Figs. 2–12) for separation

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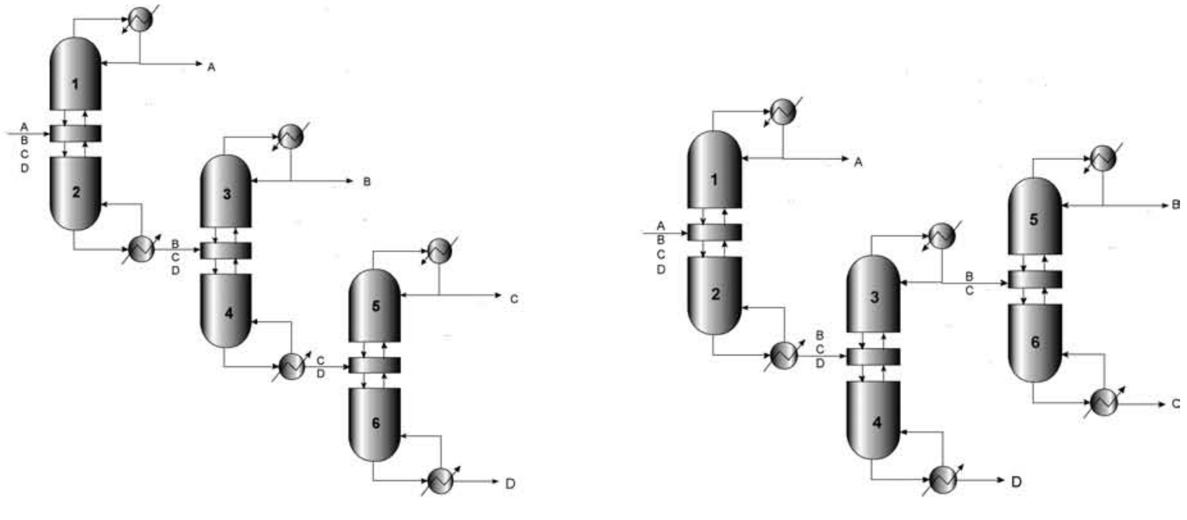
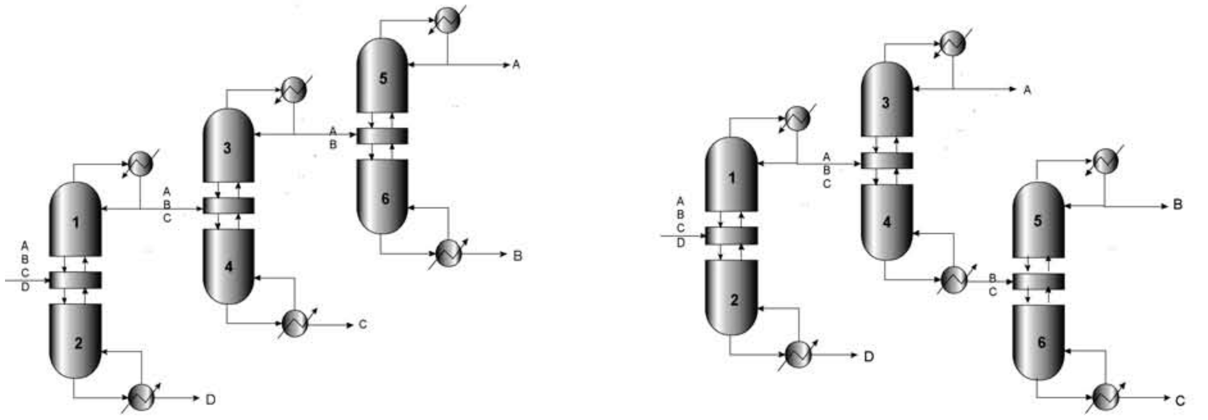


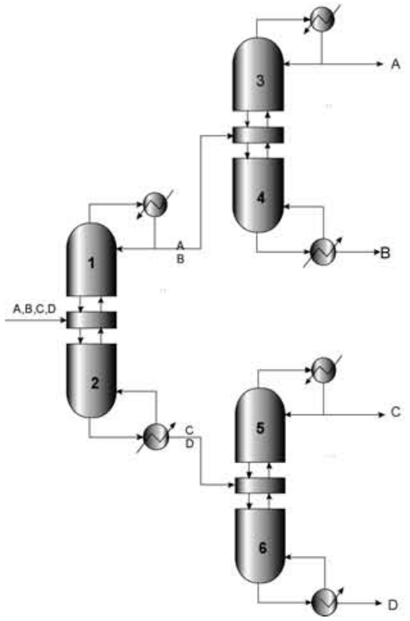
a) Conventional Sequence I (CS - I)

b) Conventional Sequence II (CS - II)



c) Conventional Sequence III (CS - III)

d) Conventional Sequence IV (CS - IV)



e) Conventional Sequence V (CS - V)

Fig. 1 – *Conventional sequences (CS) for separation of quaternary mixtures*

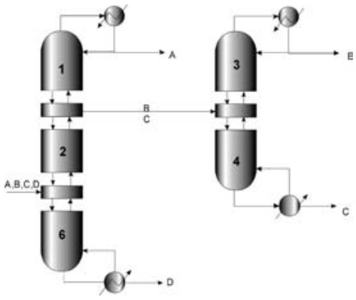


Fig. 2 – *Complex column I (CC – I)*

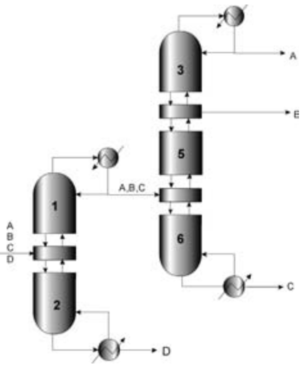


Fig. 3 – *Complex column II (CC – II)*

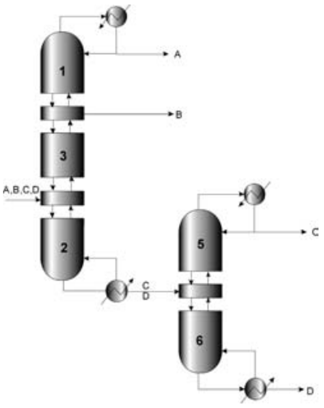


Fig. 4 – *Complex column III (CC – III)*

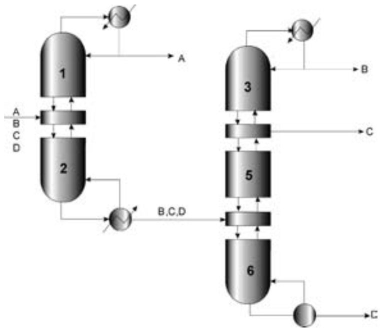


Fig. 5 – *Complex column IV (CC – IV)*

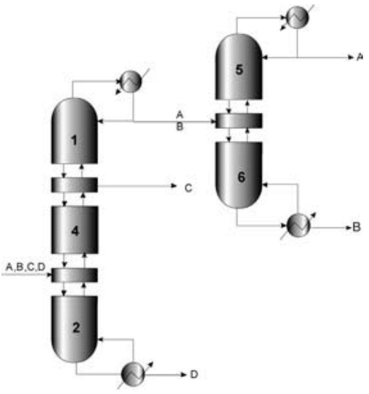


Fig. 6 – *Complex column V(CC – V)*

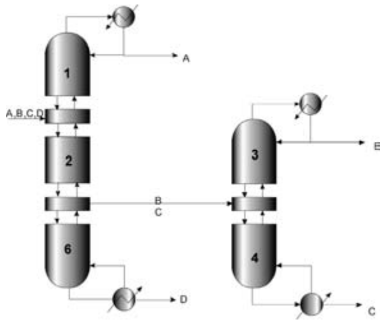


Fig. 7 – *Complex column VI (CC – VI)*

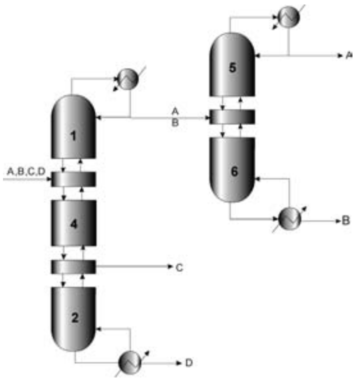


Fig. 8 – *Complex column VII (CC – VII)*

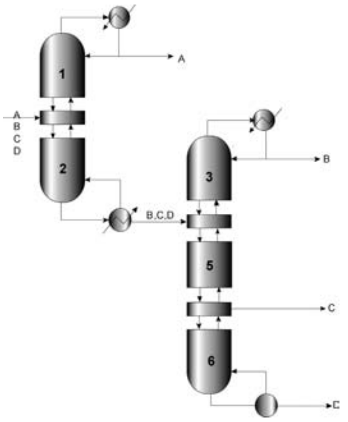


Fig. 9 – *Complex column VIII (CC – VIII)*

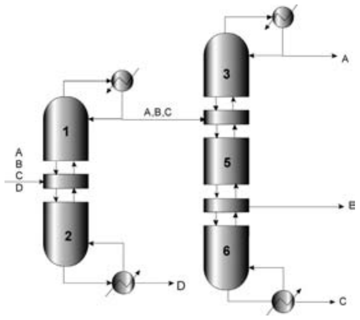


Fig. 10 – *Complex column IX (CC – IX)*

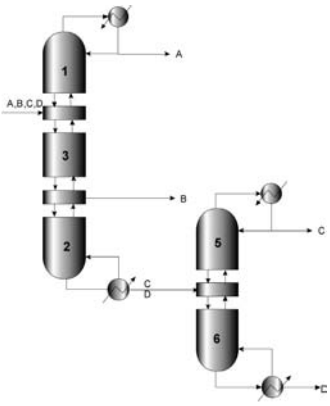


Fig. 11 – *Complex column X (CC –X)*

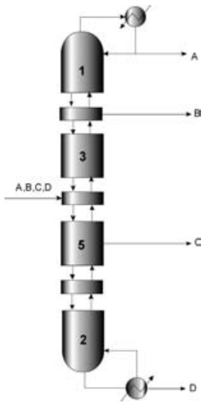


Fig. 12 – *Complex column XI (CC – XI)*

of quaternary mixtures. The results were compared to five base cases with three columns each (Fig. 1). Some rules are presented to predict which sequence will have the lowest energy consumption capital cost and better dynamic properties.

Design of complex schemes

The design of arrangements with less than N-1 columns could be modeled through superstructures suitable for optimization procedures. In these lines, two efforts for the optimal design of complex distillation columns must be mentioned: the works of Yeomans and Grossmann[5] and Barttfeld *et al.*[11] In this work, we presented an energy-efficient design procedure for the design of complex arrangements. To overcome the complexity of the simultaneous solution of the tray arrangement and energy consumption within a formal optimization algorithm, we decoupled the design problem in two stages: (1) tray configuration; (2) optimal energy consumption.

In the conventional sequences, each column performs its respective split (i.e. the separation of the light and heavy key components) with a recovery of 98 %. Using the well-known short cut methods of Fenske-Underwood and Gilliland, the tray structure of conventional distillations schemes was obtained. The number of the trays was obtained using a reflux ratio of 1.33 times the minimum value for each separation.

The first stage of our approach begins with the development of preliminary designs for the complex systems from the design aspects on conventional distillation columns: similar procedure to the design of thermally coupled distillation sequences (Hernández and Jiménez[23]). The conventional sequences (Fig. 1) show six different tray sections. These sections were used as a basis for the arrangement of the tray structure of the coupled schemes through a section analogy procedure. For instance, in the main column of the complex sequence of Fig. 2, the total number of trays was obtained by conceptually moving the stripper section from the third column to the bottom of first column of conventional sequence – I (Fig. 1a). The total number of trays in the second column of the complex sequence is equal to the stages in the second column of the conventional arrangement. Section number 5 was not used. This situation generates an arrangement with less than N-1 columns to base cases with three columns. A similar procedure was applied to obtain the other complex schemes.

After the tray arrangement for the arrangement with less than N-1 columns designs had been obtained, an optimization procedure was used to minimize the heat duty supplied to the reboilers of each complex scheme, taking into account the constraints imposed by the required purity of the four products streams. Then, the degrees of freedom that remain, after using the design specifications and tray arrangement to obtain the operating conditions, were used to obtain the integrated designs that provide minimum energy consumption. Two degrees of freedom remain for each complex sequence. They are the side stream flow and the side stream stage.

The optimization strategy can be summarized as: (a) A base design for the complex schemes is obtained. (b) A value for each side stream stage and flow is assumed. (c) A rigorous model for the simulation of complex schemes with the proposed tray arrangement is solved. In this work we used Aspen Plus 11.1™ for this purpose. If the product compositions are obtained, then the design is kept; otherwise, proper adjustments must be made. (d) One value of side stream flow is changed, going back to step (c) until a local minimum in energy consumption for the assumed value of side stream stage is detected. (e) The value of side stream stage is modified, going back to step (c) until the energy consumption is minimum. This result implies that an optimum value has been detected for the design of the complex schemes (representative example in Fig. 13).

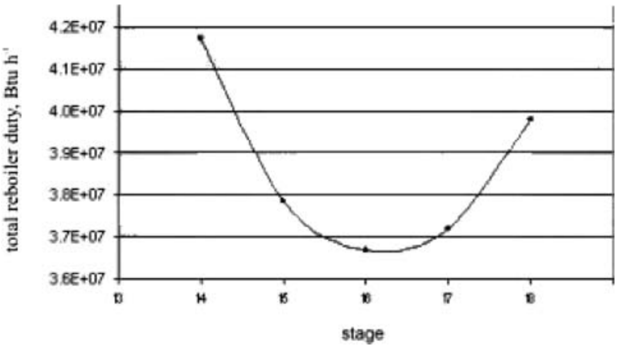


Fig. 13 – *Search for energy – efficient design in function of the side stream stage position (case CC – VIII)*

Cost estimation

For a given number of theoretical trays, Aspen Plus simulator calculates column diameter and height (for 24 in tray spacing) after converging for selected valve tray column with 2 in weir height. Valve trays of Glitsch type are considered. The costing of distillation column (carbon steel construction) was estimated by the cost equations shown in Turton *et al.*[24] that are updated with the CEPCI (Chemical Engineering Process Cost Index). The total column cost is the sum of the installed cost of column shell and the installed cost of column trays. On the other hand, the size and cost of heat exchangers were calculated. The cost of heat exchangers can be correlated as a function of the surface area assuming shell and tube, floating head, and carbon steel construction. The installation prices are updated by the CEPCI index. The capital cost (purchase plus installation cost) is annualized over a period which is often referred to as plant life time:

$$\text{Annual capital cost} = \frac{\text{Capital cost}}{\text{Plant life time}} \qquad (1)$$

$$\text{Total annual cost (TAC)} = \text{Annual operating cost} + \text{Annual capital cost} \qquad (2)$$

Operating costs were assumed just utility cost (steam and cooling water).

Plant life = 5 years

Operating hours = 8400 h yr^{-1}.

Control properties

One of the basic and most important tools of modern numerical analysis is the Singular value decomposition (SVD). There are numerous important applications of the SVD when quantitative and qualitative information is desired about linear maps. One important use of the SVD is in the study of the theoretical control properties in chemical process. One definition of SVD is:

$$G = V\,\Sigma W^H \qquad (3)$$

Here, G is the matrix target for SVD analysis, Σ is a diagonal matrix which consists of the singular values of G, V is a matrix which contains the left-singular vector of G and W is the matrix composed by the left-singular vectors of G (Klema and Laub[25]).

In the case where the SVD is used for the study of the theoretical control properties, two parameters are of interest: the minimum singular value (σ_*) the maximum singular value (σ^*), and its ratio known as condition number (γ):

$$\gamma = \frac{\sigma^*}{\sigma_*} \qquad (4)$$

The minimum singular value is a measure of the invertibility of the system and represents a clue of potential problems of the system under feedback control. The condition number reflects the sensitivity of the system to uncertainties in process parameters and modelling errors. These parameters provide a qualitative assessment of theoretical control properties of the alternate designs. The systems with higher minimum singular values and lower condition numbers are expected to show the best dynamic performance under feedback control. In the case of the condition number the best option would be values near to the unit (Klema and Laub[25]). Also, it is important to note that a full SVD analysis should cover a wide range of frequencies.

The SVD technique requires a transfer function matrix [G in eq. (3)] around the optimum design of the distillation sequences, and registering the dynamic responses of products composition. For the distillation sequences presented in this work, four controlled variables were considered, the products composition A, B, C, and D. Similarly, four manipulated variables were defined, reflux ratios (R_j) and heat duties supplied to reboilers (Q_j), depending on the structure. For example in the case CS – I we use the reflux ratio, where are obtained A, B and C and heat duty in the other component (see, for instance, a similar case of study in Segovia-Hernández *et al.*[26]). The Table 1 show the transfer function matrix (G) for CS – I. It can be noted that the dynamic re-

Table 1 – *Transfer function matrix for CS – I (M1)*

	Reflux ratio 1	Reflux ratio 2	Reboiler duty 1	Reflux ratio 3
A	$\frac{0.0126}{1+0.6280s}$	$\frac{-3e^{-0.5S}}{(1+0.0015s)(1+2.1516s)}$	$\frac{-0.0003}{1+2.2502s}$	$\frac{0.0127}{1+0.4828s}$
B	$\frac{0.0231e^{-0.125S}}{1+0.2525s}-\frac{-0.0034}{1+1.42s}$	$\frac{0.0076}{1+0.3583s}$	$\frac{-0.0109}{1+0.3388s}$	$\frac{-0.0055}{1+0.5245s}-\frac{0.0007}{1+0.9997s}$
C	$\frac{-0.0042}{(1+0.1132s)(1+0.3556s)}$	$\frac{-0.0060}{1+0.3883s}$	$\frac{0.0046}{1+0.1828s}$	$\frac{-0.0006e^{-0.24S}}{1+0.2107s}-\frac{-0.0205}{1+(1.1299s)^2+2(1.1299)(0.8574s)}$
D	$\frac{8.5e^{-0.5S}}{1+6.8385s}$	$\frac{8.5e^{-0.5S}}{1+6.819s}$	$\frac{8.5e^{-0.5S}}{1+6.5828s}$	$\frac{0.0139}{1+0.3977s}$

sponses can be adjusted to first or second order models. Similar transfer function matrix can be obtained for all cases of study.

Case of study

The case studies were selected to reflect different separation difficulties and different contents of the intermediate component of the quaternary mixtures. The mixtures considered are displayed in Tables 2–3. The mole fraction of 0.05 was shown to be a borderline value for use of side-stream columns for ternary separations (Tedder and Rudd[1]). The specified product purity for components A, B, C and D were 98.7, 98, 98 and 98.6 %, respectively. When a side-stream system has economics approximately equal to those of a base case, it will become more favorable with lower feed concentrations and less favorable with higher feed concentrations (Kin and Wankat[22]). On the basis of the ternary study (Tedder and Rudd[1]), the side-stream configurations in Figs. 2–6, which have liquid side streams withdrawn above the feed, may be desirable when the feed contains little A and significant amounts of B (Figs. 2–4), little B and significant amounts of C (Fig. 5), or little A plus B and significant amounts of C. The cascades shown in Figs. 7–11, which have vapor side streams withdrawn below the feed, may be favorable when the feed contains little D and large amounts of C (Figs. 7–9), little C and large amounts of B (Fig. 10), or small amounts of C plus D and large amounts of B. The single column shown in Fig. 12 is a special case that may be applicable when the feed contains little A and little D, but significant amounts of B and C. The total feed flow rate for all cases was 45.5 kmol h^{-1}. Since the feed involves a hydrocarbon mixture, the Chao-Seader correlation was used for the prediction of thermodynamic properties. The design pressure for each sequence was chosen such that all condensers could be operated with cooling water.

Results

We consider the almost ideal quaternary systems containing four of the five components *n*-butane, *n*-pentane, *n*-hexane, *n*-heptane, and *n*-octane with variable feed concentrations. The performance analysis is based on comparison of the operating, capital costs and dynamic properties. The tray arrangements and some important design variables for some representative sequences after the optimization task are given in Tables 4–5.

Energy consumption and TAC

For the mixtures listed in all examples (Tables 2–3) the respective configurations are evaluated on the basis of the summation of reboiler duties and the total annual cost.

From the simulation result for the case M1 (Tables 6 and 8) the system CS – III requires the least TAC (and energy consumption). The base case shown in Fig. CS – IV is next and requires a significantly higher TAC. The purities of all products can be improved by adding more stages for both base cases. Tables 7 and 9 display the simulation results for example M1 for saturated liquid side-stream cascades (Figs. 2–6) and for saturated vapor side-stream cascades (Figs. 7–11). Since there is little A in the feed, we expect the saturated liquid side-stream systems (Figs. 2–6) to in general be better than saturated vapor side streams (Tedder and Rudd[1]) The TAC and energy consumption values confirm this conclusion (schemes CC – I to CC – V have the lowest values in comparison with configurations CC – VI to CC – X). On the basis of the results the configurations CC – II and CC – III are the best of the side-stream configurations (they have similar values of TAC and reboiler duty). They require similar heating to the best base cases, and TAC is similar to the best conventional sequences. However, the conventional sequences are more flexible if the concentration of A in the feed increases. In this case, a more detailed dynamic behavior study would be justified.

Case M2 has little middle component B in the feed mixture, and A/B, B/C, and C/D splits are of approximately equal difficulty. Using the Heuristics by Tedder and Rudd[1] the best side-stream configuration is that in Fig. 5. However, since this is a quaternary separation, in this case, the best option is CC – IV. Compared to the conventional sequence cases (Fig. 1), the configuration CC – IV requires the least heating and it has the least TAC value.

Tables 6–9 show simulation results for the case M3. The CC – V scheme has the largest capital cost. The configuration CC – VII has the least overall energy use and TAC value. The effects of little presence of components A and D are explored in this case. For this example, saturated vapor side-stream cascade is the best option.

Table 9 shows simulation results of M4 for configurations shown in Fig. 1. Case of study M4 has little component A in the feed mixture, and the A/B, B/C, and C/D separations are of approximately equal difficulty. From the simulation results the system shown in Fig. 1c has the best TAC. The base case shown in Fig. 1d is next and it has a significantly higher TAC.

Table 2 – *Design examples (with n-heptane)*

Component		Feed composition (kmol h^{-1})				
		M1	M2	M3	M4	M5
n-butane	A	2.56	30	5	5	30
n-pentane	B	25.64	3	45	25	40
n-hexane	C	41.03	55	45	40	25
n-octane	D	30.77	12	5	30	5

Table 3 – *Design examples (with n-octane)*

Component		Feed composition (kmol h^{-1})		
		M6	M7	M8
n-butane	A	30	5	3
n-pentane	B	40	25	55
n-hexane	C	25	40	12
n-octane	D	5	30	30

Table 4 – *Design variables for the CS – I, M1*

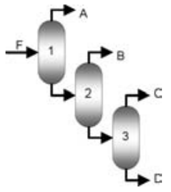
	Column 1	Column 2	Column 3
number of stages	19	19	23
feed stage	11	11	12
distillate flow rate, kmol h^{-1}	2.5	25.5	40.9984756
bottom flow rate, kmol h^{-1}	97.5	72	31.0015244
feed flow rate, kmol h^{-1}	100	97.5	72
reflux ratio	31.9048632	4.09584664	2.05830395
temperature of distillate, K	342.804476	323.204607	342.804476
pressure of top, bar	4.5	1.5	1.0
diameter, m	0.66053268	0.91061622	1.03004497

Table 5 – *Design variables for the CC – I, M1*

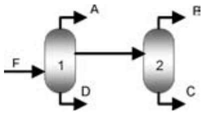
	Column 1	Column 2
number of stages	30	19
feed stage	19	11
side – stream stage	12	–
distillate flow rate, kmol h^{-1}	2.22511543	26.027885
bottom flow rate, kmol h^{-1}	30.4748846	41.272115
feed flow rate, kmol h^{-1}	100	67.2
side-stream flow rate, kmol h^{-1}	67.2	
reflux ratio	159.859537	5.03505221
temperature of distillate, K	322.199744	322.293627
pressure of top, bar	4.5	1.5
diameter, m	1.30410259	1.00603716

Table 6 – *Some energy consumption of conventional sequences*

Sequence	Reboiler duty (cal s^{-1})			
	M1	M2	M3	M6
CS – I	1,071,912.34	1,130,136.32	1,035,793.08	756,127.61
CS – II	1,086,690.37	1,133,977.50	1,463,727.68	862,836.18
CS – III	942,147.42	1,180,394.52	1,121,378.85	1,139,274.56
CS – IV	990,930.59	1,110,803.90	1,254,850.37	993,116.76
CS – V	1,063,502.94	1,031,456.54	962,192.03	784,948.18

Table 7 – *Some energy consumption of complex sequences*

Sequence	Reboiler duty (cal s^{-1})			
	M1	M2	M3	M6
CC – I	1,441,340.15	56,937,032.18	1,404,166.54	4,989,243.45
CC – II	1,044,272.54	4,203,484.35	1,518,022.22	3,905,320.32
CC – III	1,083,787.46	4,895,575.91	1,227,898.14	7,032,081.32
CC – IV	3,810,956.44	867,291.12	6,414,701.98	6,032,453.68
CC – V	3,930,214.26	2,300,712.94	6,685,032.69	7,789,548.03
CC – VI	8,001,298.50	2,706,645.45	1,673,415.32	809,977.39
CC – VII	4,832,395.03	2,517,592.46	819,269.86	697,336.90
CC – VIII	5,098,972.89	1,861,802.17	1,010,732.17	666,168.67
CC – IX	5,712,017.34	7,912,878.41	6,090,935.15	3,438,816.43
CC – X	6,866,609.68	8,080,458.26	6,325,321.73	3,314,651.38
CC – XI	8,441,309.40	4,034,366.26	1,740,801.13	3,474,282.94

Table 8 – *Total annual cost (TAC) of conventional sequences*

Sequence	TAC ($\$\ \mathrm{yr}^{-1}$)							
	M1	M2	M3	M4	M5	M6	M7	M8
CS – I	601,947	645,023	582,454.15	623,278	486,400	446,710	520,157	536,760
CS – II	623,559	656,493	785,273.16	747,527	563,655	529,545	518,068	615,943
CS – III	577,705	723,399	676,066.41	582,685	697,320	765,154	562,579	554,983
CS – IV	605,981	673,046	733,544.97	613,509	648,547	635,012	561,203	505,911
CS – V	610,821	594,068	563,988.12	630,563	558,486	483,821	444,550	553,821

Table 9 – *Total annual cost (TAC) of complex sequences*

Sequence	TAC ($\$\ \mathrm{yr}^{-1}$)							
	M1	M2	M3	M4	M5	M6	M7	M8
CC – I	828,872.06	28,905,388.81	852,565.07	941,387	2,870,535	2,973,460.81	893,688	514,305
CC – II	630,654.47	1,926,381.71	866,828.81	709,899	2,008,619	2,001,789.26	586,255	552,818
CC – III	603,482.35	2,394,265.24	669,752.27	639,838	1,967,664	3,345,151.43	562,308	535,545
CC – IV	1,879,893.90	512,954.14	3,092,905.74	1,840,449	2,818,330	3,200,586.60	1,950,935	3,873,796
CC – V	1,983,838.18	1,373,682.21	3,275,641.50	1,960,644	3,721,500	4,755,711.16	2,157,940	4,342,479
CC – VI	4,191,186.82	1,522,286.18	961,497.67	3,944,359	1,078,162	548,532.92	1,668,124	2,964,713
CC – VII	2,429,521.00	1,510,347.68	543,664.14	2,532,203	599,110	537,414.64	887,410	991,513
CC – VIII	2,497,922.23	1,038,970.09	600,804.07	2,372,364	623,161	433,435.05	918,141	1,018,244
CC – IX	2,812,094.48	3,802,706.46	3,000,633.57	2,713,809	1,784,706	1,810,688.08	2,605,430	956,870
CC – X	3,521,690.36	3,843,641.98	3,044,146.79	3,267,508	2,187,407	1,672,180.77	2,841,512	3,839,664
CC – XI	4,523,731.83	2,291,865.71	1,053,963.33	4,081,785	2,202,311	2,199,070.68	2,250,913	1,640,116

Table 9 shows the simulation results for example 1 for saturated liquid side-stream cascades and for saturated vapor side-stream cascades (Figs. 2–6 and 7 and 9–11, respectively). Unlike the base case, it is difficult to increase the purity of the side stream product B or C since A or D is always present when it is withdrawn. Since there is little A in the feed, we expect the saturated liquid side-stream systems (Figs. 2–6) to in general be better than saturated vapor side streams. The results confirm this. On the basis of the simulation results, the configuration CC – III is the best of the side-stream configurations. It requires significantly less heating than the base case (Fig. 1), but capital costs are higher than that of the base cases.

Tables 8 and 9 display results for mixture M5. Since there is very little component D in the feed flow rate, the base cases and the configurations in Figs. 7–11 with saturated vapor side streams are studied. The direct sequence (Fig. 1a) and indirect sequence (Fig. 1b) have the lowest TAC. The configurations shown in Figs. 8 and 9 have the lowest operation cost. In this case the conventional and complex sequences have similar TAC values.

To explore the effect of the components in the feed, the *n*-heptane was replaced with *n*-octane.

Example M6 has an easy C/D separation and small amounts of D, the vapor side-stream systems in Figs. 7–9 are studied. Tables 6–9 show the simulation results. The configuration CC – VIII clearly has the lowest operating cost and capital cost when it is compared with all conventional sequences (Fig. 1). We can compare example M6 to example M5, which has the same feed mole fractions, but component D is *n*-octane. The best side-stream configuration was CC – VII, but the conventional sequence (Fig. 1a) was best. The easier separation in example M6 favors the side-stream system.

Tables 8 and 9 show the results for M7 and M8, which contain very little component A in the feed mixture. According to the simulation results, the configuration CC – III is clearly the best of the side-stream configurations for example M7. Compared to the best conventional sequence (Fig. 1e), the configuration CC – III has similar value of TAC. For case M8, which contains more B and less C, the configuration CC – I has similar TAC to conventional sequence CC – IV.

Dynamic properties

A full SVD analysis should cover a sufficiently complete range of frequencies. For this initial analysis of complex configurations, we simply estimated the SVD properties for each separation system at zero frequency. Such analysis should give some preliminary indication on the control properties of each system around the nominal operating point.

Tables 10 and 11 give the results for the SVD test for each sequence (case M1). In the case of conventional sequences the CS – V has the best values. In the case of the complex sequences, the schemes CC – II and CC – III show the best results, which imply that those sequences are better conditioned to the effect of disturbances than the other complex systems. Those results show that the saturated liquid side-stream systems have better dynamic behavior. This situation is similar to the TAC values for the case M1, since there is little A in the feed.

The control properties for M2 are displayed in Tables 12 and 13. The conventional sequences CS – II and CS – V show the best value for γ and σ^*. In the case of the complex sequences, the scheme CC – V shows better dynamic behavior. Therefore, it can be expected that those complex systems exhibit better control properties under feedback control. In this case the better complex sequence does not have the lowest TAC value.

Table 10 – *Minimum singular value and condition number for each structure (M1)*

Sequence	σ_*	γ
CS – I	0.0027403	979.6
CS – II	0.023851	594.6
CS – III	9.5833E–05	9,889.1
CS – IV	0.0072318	210.8
CS – V	0.015673	280.9

Table 11 – *Minimum singular value and condition number for each structure (M1)*

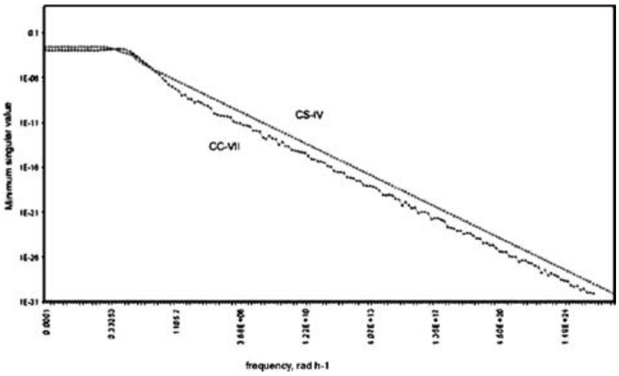
Sequence	σ_*	γ
CC – I	0.00014653	20,714.5
CC – II	0.0023106	487.7
CC – III	0.0055807	552.7
CC – IV	0.0016101	9,591.3
CC – V	0.00020189	121,387.8
CC – VI	8.7115E–11	43,860,414,394.7
CC – VII	0.0013788	4,235.4
CC – VIII	0.0015073	6,429.5
CC – IX	0.0011245	1,843.9
CC – X	4.5061E–07	14,924,657.6
CC – XI	0.0008959	5,970.1

Table 12 – *Minimum singular value and condition number for each structure (M2)*

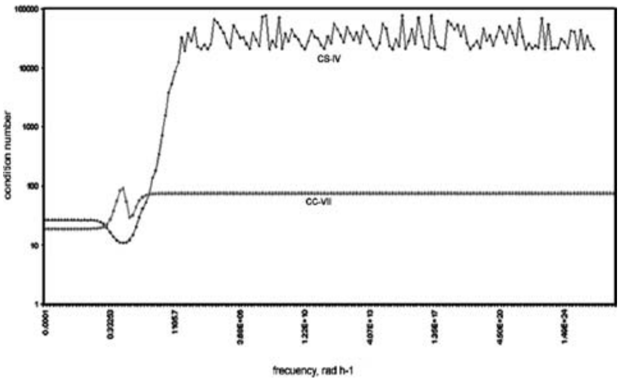
Sequence	σ_*	γ
CS – I	0.00010146	50,209.9
CS – II	0.010959	3,727.3
CS – III	0.000516	4,586,821.7
CS – IV	0.0025804	21,163.3
CS – V	0.012568	2,582.5

Table 13 – *Minimum singular value and condition number for each structure (M2)*

Sequence	σ_*	γ
CC – I	2.9107E–07	4,699,556.8
CC – II	0.001512	3,296.6
CC – III	0.00022212	1,595,623.9
CC – IV	0.0024763	316,124.8
CC – V	1.868	44.1
CC – VI	1.4209E–05	32,446,336.8
CC – VII	0.0078564	7,412.5
CC – VIII	0.0019278	263,569.8
CC – IX	0.0013733	3,637.2
CC – X	0.00013312	70,965.3
CC – XI	0.0012256	8,888.7



F i g . 1 4 – *Minimum singular value CS – IV and CC – VII (M3)*



F i g . 1 5 – *Condition number CS – IV and CC – VII (M3)*

The results for the condition number and minimum singular value, for case M3 (Tables 14 and 15) show that the conventional sequence CS – IV offers the best values. When we studied the complex sequences, the better dynamic behavior results can be observed in scheme CC – VII. As a result, it can be expected that those distillation systems are better conditioned to the effect of disturbances than other configurations. Figs. 14 and 15 show values of σ^* and condition number for the whole frequency range for CC – VII and CS – IV. Therefore, the complex scheme is expected to require similar effort control under feedback operation and it is conditioned to the effect of disturbances similar to CS – IV sequence. The CC – VII has the least overall energy use and TAC value. In this case the CC – VII is the better option.

The results for case M6 are shown in Tables 16 and 17. The sequences CS – III, CS – IV and CC – V have similar values for γ and σ_*, they have

T a b l e 1 4 – *Minimum singular value and condition number for each structure (M3)*

Sequence	σ_*	γ
CS – I	8.9039E–05	29,282.6
CS – II	0.00017842	16,923.5
CS – III	0.002752	1,289.1
CS – IV	0.003176	593.9
CS – V	6.0317E–05	6,915.9

T a b l e 1 5 – *Minimum singular value and condition number for each structure (M3)*

Sequence	σ_*	γ
CC – I	0.00044799	5,771.3
CC – II	0.00045169	7,923.7
CC – III	0.0021578	5,693.3
CC – IV	0.0015473	2,673.5
CC – V	4.1848E–05	97,316.5
CC – VI	0.00051199	6,859.5
CC – VII	0.015939	200.8
CC – VIII	4.8798E–06	752,510.3
CC – IX	0.0013472	2,732.7
CC – X	2.8225E–05	851,018.6
CC – XI	0.0011972	15,040.9

T a b l e 1 6 – *Minimum singular value and condition number for each structure (M6)*

Sequence	σ_*	γ
CS – I	0.0015384	20,434.8
CS – II	0.0061419	453.3
CS – III	0.0072285	266.5
CS – IV	0.0078083	180.7
CS – V	0.0040689	932.8

T a b l e 1 7 – *Minimum singular value and condition number for each structure (M6)*

Sequence	σ_*	γ
CC – I	0.0011715	22,206.5
CC – II	0.001564	6,258.7
CC – III	2.5501E–07	172,906,944.8
CC – IV	0.0015687	2,528.1
CC – V	0.036755	112.6
CC – VI	0.00093487	51,760.1
CC – VII	0.021396	1,526.3
CC – VIII	0.0083498	4,112.4
CC – IX	0.0013305	11,285.2
CC – X	0.00011775	116,492.5
CC – XI	0.001634	6,189.1

the best dynamic properties (higher values of σ^* and lower values of condition number). Therefore, it can be expected that the conventional and complex systems exhibit similar control properties under feedback control and they are better conditioned to the effect of disturbances. In this case the complex sequence does not have the lowest TAC value. Similar results can be shown for the other mixtures in the case of the control properties.

Overall results

Based on the trends observed, we can propose two heuristics (similar to the Kim and Wankat's rules, 2004) for the use of complex sequences taking into consideration TAC values and dynamic behavior:

(a) Use a complex scheme with a liquid side stream above the feed if there is a small amount (approximately 0.05 mole fraction or less) of the most volatile component in the feed.

(b) A complex scheme with a vapor side stream below the feed can be used if there is a small amount (approximately 0.05 mole fraction) of the least volatile component in the feed to this column.

Conclusions

A comparative study of the TAC values and theoretical control properties of the side-streams designs with less than N-1 columns for quaternary distillations has been conducted. The alternative arrangements emerge from a reduction in the number of sections in the structure of conventional sequences. A general energy-efficient design procedure is developed for any type of the side-streams designs with less than N-1 columns. The method is based on a section analogy procedure with respect to the characteristics of a conventional distillation sequence. The methodology provides a robust tool for the design of multicomponent side-streams designs. The examples have shown that the design procedure can provide all of the operating parameters needed. Some trends were observed for the use of complex sequences: the best option in TAC values and dynamic properties for complex schemes with a liquid side stream above the feed is when there is a small amount (approximately 0.05 mole fraction or less) of the most volatile component in the feed. The case of complex scheme with a vapor side stream below the feed is when a small amount (approximately 0.05 mole fraction) of the least volatile component is in the feed to this column. In the other cases, the best options are the conventional sequences.

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List of symbols

G – transfer function matrix
N – number of column
V – matrix of left eigenvectors
W – matrix of right eigenvectors
γ – condition number
Σ – diagonal matrix
σ^* – maximum singular value
σ_* – minimum singular value

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