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Controllability analysis of heat integrated distillation systems for a multicomponent stream

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ABSTRACT

Understanding the dynamic behavior of distillation columns has received considerable attention due to the fact that distillation is one of the most widely used unit operations in chemical process industries. Heat integrated distillation sequences can provide significant energy savings; however, they exhibit a complex structure which appears to affect their controllability properties. One potential solution to this problem has been suggested through the operation of heat integrated sequences under the conditions that do not provide minimum energy requirements. But, this work proved that the process under the conditions of minimum energy requirements can operate with the best controllability properties. In this work, the controllability properties were analyzed with the application of the Morari resiliency index, condition number and relative gain array, which were frequency-dependent indices. The results showed that the controllability of the best heat integrated distillation column with the minimum total annual cost was better than other sequences.

1. Introduction

Certainly, distillation is the most widely applied separation technology and will continue as an important process for the foreseeable future because there seems not to be another industrially viable alternative around. Although distillation is generally recognized as one of the best developed chemical processing technologies, there are still many barriers that could, when being overcome, secure the position of distillation and even make it more attractive for use in the future. The main disadvantage of distillation is its high-energy requirements. Appropriate integration of the distillation column with the overall process can result in significant energy savings, but the scope for this is often limited. The classical design of a distillation system for a multicomponent separation uses only the simple columns. Each of the simple columns in a multicomponent distillation configuration receives a feed and performs a sharp split between two adjacent components of the feed mixture. The simple column configurations for multicomponent distillation are easy to design and operate. Because the number of separation sequences increases dramatically when the number of components in the feed mixture increases, a considerable number of works have been conducted on the optimal synthesis of simple column configurations for an n component separation. Thompson and King reported the following formula for calculating the number of all simple configurations (King, 1980):

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

where S_n is the number of sequences and n is the number of component in the feed stream. The task for designing a heat integrated simple column configuration consists of searching for the possible heat matches among all of the condensers and rebuilders of the simple columns. Rev, Emtir, Szitkai, Mizsey, and Fonyo (2001) provided a comprehensive study on the energy saving for ternary systems. Separation configurations, internal thermal coupling and external heat integration were explored. A large number of studies have been done for the synthesis of the optimal heat integrated simple column configurations since the works done by Rathore, Wormer, and Powers (1974), Dhallu and Johns (1988), Schuttenhelm and Simmrock (1992) and Errico, Rong, Tola, and Turunen (2009). Lots of works in this area have tried to find a better heat integrated sequence for ternary mixture streams which consist of 24

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Nomenclature

A	area of heat transfer in heat exchanger
a	year
BU3	boil up ratio of column 3
BU2	boil up ratio of column 2
$C()$	total annual cost model for the system
CN	condition number
C1	condenser of column 1
C2	condenser of column 2
C3	condenser of column 3
CW	cooling water
D	diameter of column
G	transfer function matrix
H	height of column
HX	heat exchanger
K	Kelvin
Min	minimum
M&S	Marshall and Swift cost index
MRI	Morari resiliency index
MWHC	molecular weight of heaviest component
Nt	number of trays
n	number of components
P	pressure
$\{p\}$	decision pressure parameter
Q	heat flow rate
R1	reboiler of column 1
R2	reboiler of column 2
R3	reboiler of column 3
RR2	reflux ratio of column 2
RR3	reflux ratio of column 3
RV	rectify vapor flow rate
RGA	relative gain array
SQP	successive quadratic programming
S_n	number of simple sequence
SVD	singular value decomposition
TAC	total annual cost
TBP	boiling point temperature
U	heat transfer coefficient of heat exchanger
V	matrix of left singular vectors
W	matrix of right singular vectors
X_i	mole fraction
$\Delta T_{\min}$	minimum temperature difference
ΔT_{LMTD}	logarithmic minimum temperature difference
ΔP	pressure difference
λ	diametrical array
σ	singular value
σ^*	maximum singular value
σ^*	Morari resiliency index

columns, 2 condensers and 2 reboilers. Considering the separation of a stream with more than 3 components extremely increases the number of different sequences and number of condenser and reboiler in the sequences which cause a large amount of different heat integration between the columns. The design, optimization and control of such energy-integrated distillation columns require engineering experience and knowledge, which represents a challenge to the researches (Bildea & Dimian, 1999; Fisher, Doherty, & Douglas, 1988; Hernandez & Jimenez, 1999; Jimenez, Hernandez, Montoy, & Zavala Garcia, 2001). In practice, the economic potential of such energy-integrated schemes has been already recognized, but their control properties have not been studied to the same degree. Since dynamic behavior and control of these heat integrated sequences are also important, recent efforts have contributed to the understanding of dynamic properties of these sequences (Abdul Mutalib & Smith, 1998; Lin & Yu, 2004; Mizsey, Hau, Benko, Kalmar, & Fonyo, 1998; Skogestad, 1997; Weitz & Lewin, 1996). Some works have studied the control for three different heat integration configurations: feed-split, light-split forward (integration) and light-split reverse (Chiang & Luyben, 1988; Han & Park, 1996). Controllability analysis of seven distillation sequences for the separation of ternary and more mixtures using singular value decomposition and closed-loop responses under the feedback control has been presented in many studies (Gabriel et al., 2007; Jimenez et al., 2001; Mc-Conville et al., 2006). The results have shown that nonconventional distillation sequences such as thermally coupled distillation sequences can have better control properties than non-integrated schemes such as conventional direct and indirect sequences, distillation systems with side streams and sequences with three conventional distillation columns. The control properties of the considered sequences were obtained using the singular value decomposition technique at zero frequency (Mc-Conville et al., 2006). The control properties of thermally coupled distillation sequences for the separation of quaternary mixtures of hydrocarbons were compared with those of conventional distillation sequences (Carlos et al., 2005).

Understanding control properties of columns with heat integrations for separating multicomponent mixtures is an extremely important issue because designs with economic incentives often conflict with their operational characteristics. Two of the most important controllability indices are the Morari resiliency index (MRI) and condition number (CN), derived from the singular value decomposition of the transfer function (linear model). The relative gain array (RGA) is also typically used for studying the controllability of distillation systems.

This paper considered the heat integrated distillation systems for the separation of a multicomponent stream to four pure groups of products according to the minimization of the total annual costs. Also, it considered the mentioned controllability indices for selecting the best control structures and comparing the controllability of the different designed distillation arrangements.

The plant configuration considered in this study's industrial case is shown in Fig. 1A. This configuration can be classified as a distributed sequence and can be represented by the following separation task: AB/CD; A/B; C/D. Other four simple column configurations possible for this separation included the direct (A/BCD; B/CD; C/D) sequences (Fig. 2A), the direct–indirect (A/BCD; BC/D; B/C) sequences (Fig. 3A), the indirect (ABC/D; AB/C; A/B) sequences (Fig. 3C) and the indirect–direct (ABC/D; A/BC; B/C) sequences (Fig. 3E).

The process design procedure is a sequential discipline in which the control design is carried out after the plant is designed. During the plant design, a number of basic plant performance requirements have to be ensured in order to obtain a design which provides acceptable operational performance. The process design alternatives are usually judged from economic aspects alone without taking operability into account.

Operability is the ability of the plant to provide acceptable static and dynamic operational performance that includes flexibility, switchability, controllability and several other issues (Weitz & Lewin, 1996).

Switchability measures the ease of moving the process from one desired stationary point to another. Similarly, resiliency measures the degree to which a processing system can meet its design objectives despite external disturbances and uncertainties in design parameters. Controllability is the capability of a process to operate economically and safely without violating constraints and to achieve various design objectives in the presence of these uncertainties. Since controllability is an inherent property of the process itself, it should be considered at the design stage before the

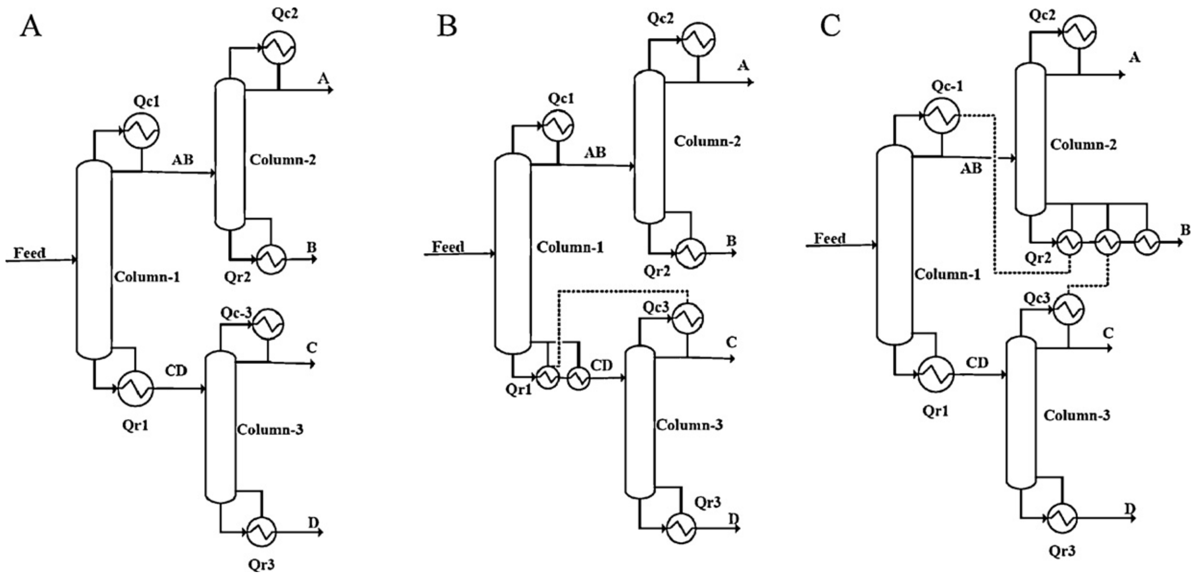

Fig. 1. Distributed sequences: A is primary distributed, B is distributed (C3–R1), and C is distributed (C1&C3–R2).

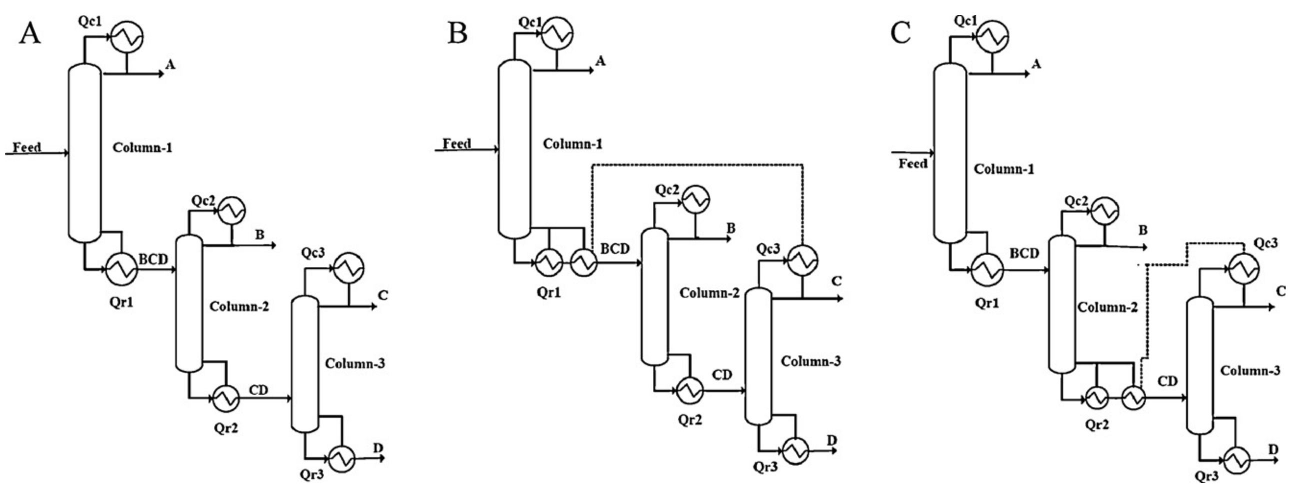

Fig. 2. Direct sequences: A is direct, B is direct (C3–R1), and C is direct (C3–R2).

control system design is fixed. The most preferable way of considering controllability at the design stage is to include controllability as one of the design objectives just like the traditional economic ones in the design optimization problem. Controllability evaluation methods may be classified to three types by the model used in the evaluation procedure, steady-state model-based, linear dynamic model-based and nonlinear dynamic model-based ones. Another way of evaluating controllability in a quantitative and explicit way is to perform dynamic simulations of the target process. However, detailed dynamic simulation requires detailed information on the system, which is not known until the later part of design stage. Hence, in the last decades, different authors (Errico et al., 2009; Gabor & Mizsey, 2008; Gabriel et al., 2007; Kencse, 2009; Lin & Yu, 2004; Mc-Conville et al., 2006) have developed simple controllability study methods, which can be carried out in the early design phase.

In addition, it is important to emphasize that the controllability analysis usually is applied for two type of problem: (i) Selection of the best controlled and manipulated variable pairing within one process. (ii) Evaluation of control properties for two or more process alternatives.

The controllability analysis is carried out by calculating the transfer function matrices (G) with the CDI interface of the Aspen Dynamics. In order to carry out the controllability study, different control indices are elaborated, which are used for predicting the degree of directionality and the level of interactions in the system. These indices can be calculated in a steady state or infrequency domain. The controllability indices applied in this article whereas follows.

2. Methodology

The objective of this research was to find the best heat integrated sequence with the minimum total annual cost and to find the best controllable sequence by MRI, CN and (RGA) controllability indices for the considered industrial case study. In the first step, all the simple sequences and heat integrated sequences were designed and optimized. In the second step, the controllability of all sequences were considered and compared.

Step 1: heat integration

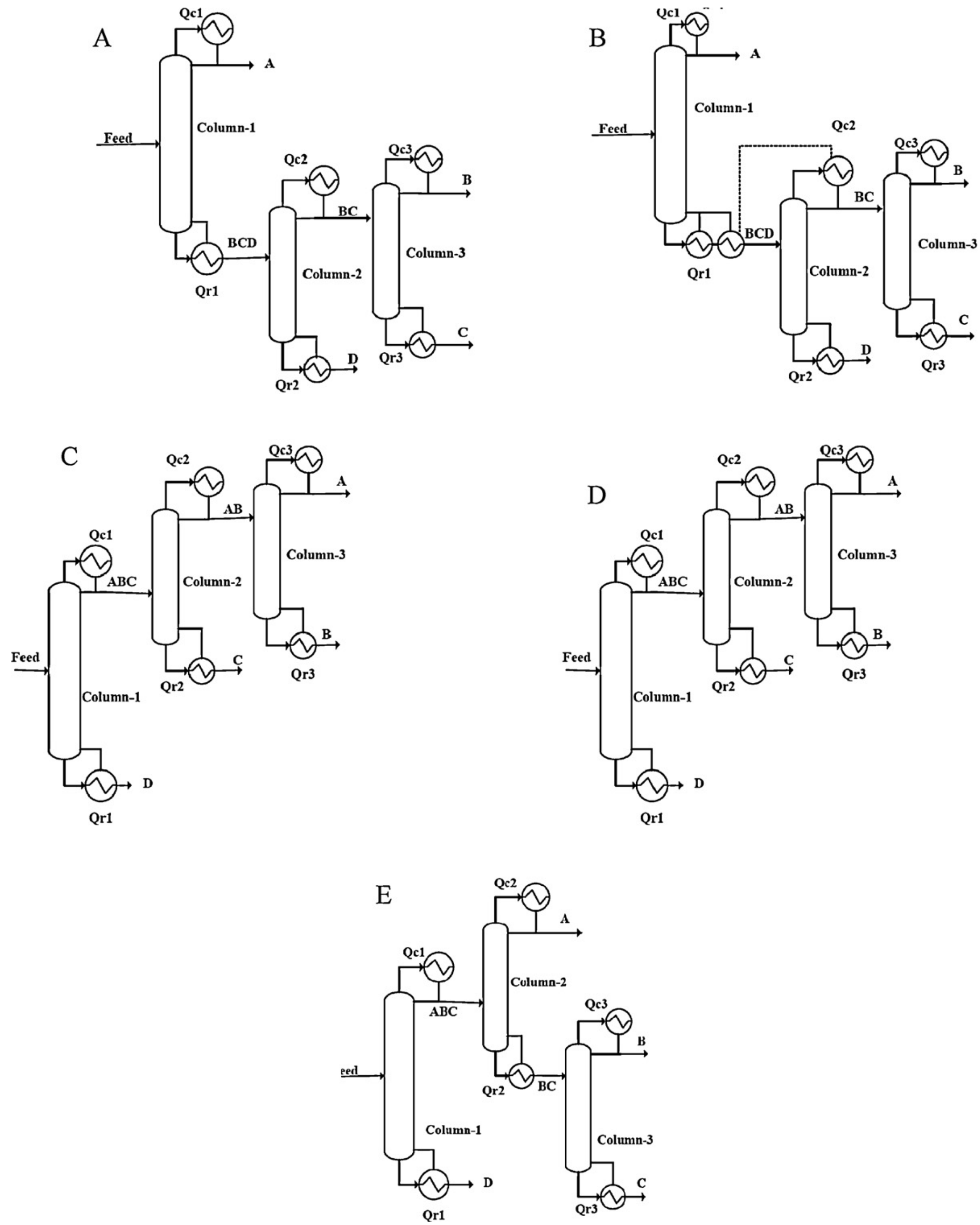

Fig. 3. Direct–indirect sequences: A is direct–indirect, and B is direct–indirect (C2–R1). Indirect sequences: C is indirect, and D is indirect (C1&C2–R3) and E is indirect–direct sequence.

In the first step, the aim was to minimize the total annual cost of sequences by creating heat integration among the columns. To calculate temperatures and heat flow rates of condensers and reboiler and to find the design specifications of columns such as the actual number of trays, reflux ratio, and rectify vapor flow, all the five simple sequences were simulated by the shortcut and rigorous method of commercial software.

Then, the equations of diameter and height of columns, annual capital cost of columns and heat exchangers and annual operation cost were modeled and used for calculating the total annual cost of each sequence. The equations used to account for the diameter and height of columns were (Emtir & Etoumi, 2009):

$$D = 5e - 3 \times \sqrt[0.25]{\mathrm{MWHC} \times (1.8 \times \mathrm{TBP} + 492)} \times \sqrt[0.5]{\mathrm{RV}} \tag{2}$$

$$H = (\mathrm{Nt} - 1) \times 0.6 + 6 \tag{3}$$

The height of column (Eq. (3)) is evaluated considering 0.6 m as tray spacing and 6.0 m as disengagement.

The basic equations for calculating the capital cost were the total cost of distillation columns and heat exchangers (Errico et al., 2009).

Table 1
Utility costs.

Utility	Temperature level (°C)	Values
LP-steam ($/t)	158	13
MP-steam ($/t)	200	16
HP-steam ($/t)	250	20
Cooling water ($/t)	35–45	0.082

The total cost of a distillation column can be considered as the sum of the costs of column shell and trays. The equation for calculating the column shell was:

$$\$\left(\frac{\text{M\&S}}{280}\right)(937.61)D^{1.066}H^{0.802} \tag{4}$$

All the correlations are valid for carbon steel construction and are updated from mid-1968 to 2009 utilizing the Marshall and Swift cost index (Chemical Engineering Magazine, 2009). The correlation (Eq. (4)) is valid for a pressure less than 345 kPa; otherwise a correction factor $\lfloor 1+1.45\times10^{-4}(P-345)\rfloor$ must be applied.

To calculate the cost of column's trays, considering sieve trays, the following correlation was utilized:

$$\$\left(\frac{\text{M\&S}}{280}\right)(97.24)DH^{0.802} \tag{5}$$

The heat exchanger cost evaluation was based on the heat exchanger area evaluated utilizing the usual design formula:

$$A = \frac{Q}{U\Delta T_{\text{LMTD}}} \tag{6}$$

Mean values of 1800 W/(m^2 K) and 2100 W/(m^2 K) were assumed for the overall heat transfer coefficient of condensers and reboilers, respectively. Assuming shell and tube, floating head and carbon steel construction, the cost correlation was as follows:

$$\$\left(\frac{\text{M\&S}}{280}\right)(474.67)A^{0.65} \tag{7}$$

The reported correlation is valid for an exchange area range between $18.6 < A < 464.5\,\text{m}^2$. The capital cost is annualized over a period which is often referred to plant life time. In this case study the plant lifetime is 10 years.

Annual operating cost was calculated by the amount of heat flow rates of condensers and reboilers of the columns and the utility costs in Table 1 (Mascia, Ferrara, Vacca, Tola, & Errico, 2007). Heat flow rates of condensers and reboilers were calculated by simulation. The time fraction of operation for annualizing the operating cost was 8000 h/year.

In the next step, after calculating the TAC function, the optimizer toolbar of the commercial software was used for minimizing the objective function of TAC according to the continuous parameters of column's pressures and the process constraints of temperatures. The optimization method SQP of the optimizer toolbar was used for minimizing the problem. With the continuous decision for the individual columns' pressure $\{p\}$, the objective function formulation was:

$$\text{Min}\quad \text{TAC} = \min \quad C(\{p\}), \quad \{p\} \in P \tag{8}$$

where $C()$ represents the total annual cost model for the system, P is the vector of operating pressures for all individual columns in the system and P can be a set of feasible range of $\{p\}$. To minimize the TAC function of each simple sequence, the continuous parameters of column's pressures can change in the range of 1–30 bars. For temperature constraints, temperatures of columns have to be between the temperatures of cooling water and the temperature of hp steam.

After optimization of the simple sequences, in next step, start to find the possible heat integration in each sequence. In each sequence, there are 3 condensers (C1, C2, C3) and 3 reboilers (R1, R2, R3), which can transfer heat to each other according to their temperatures. For each sequence there would be 12 different situations for heat integration:

$$\begin{gathered}\text{C1}\to\text{R2},\quad \text{C1}\to\text{R3},\quad \text{C1}\to\text{R2\&R3},\quad \text{C2}\to\text{R1},\quad \text{C2}\to\text{R3},\\ \text{C2}\to\text{R1\&R3},\quad \text{C3}\to\text{R1},\quad \text{C3}\to\text{R2},\quad \text{C3}\to\text{R1\&R2},\\ \text{C1\&C2}\to\text{R3},\quad \text{C2\&C3}\to\text{R1},\quad \text{C1\&C3}\to\text{R2}\end{gathered}$$

For example, the situation C1 → R2 means that the condenser C1 transfers heat to reboiler R2, according to the minimum temperature difference $\Delta T_{\min} = 10\,\text{K}$. To find whether the condenser C1 can transfer heat to reboiler R2, we increased the pressure of column 1 to the allowable maximum pressure point, according to the temperature constraint, to increase the temperature of the condenser C1 to its maximum level. On the other side, we decreased the pressure of column 2 to allowable minimum pressure, according to the temperature constraint, to decrease the temperature of reboiler R2. If the temperature of condenser C1 was higher than the temperature of reboiler R2 plus $\Delta T_{\min}$, the heat integration of C1 → R2 could be possible. Now for this situation, a new temperature constraint ($T_{\text{C1}} - T_{\text{R2}} > 10$) and some changes to the calculation of total annual capital cost and annual operation cost are added to the optimization procedure of the objective function of TAC in optimizer toolbar. The optimum pressures of columns and the minimum TAC are obtained by the optimization and the data and structure of sequence with heat integration of C1 → R2 are stored. Totally, for all five simple sequences, there would be 60 different situations for heat integration.

This procedure is done for all the mentioned deferent situation of heat integration for each simple sequence and all the possible heat integrated sequences are optimized. Finally, the optimum simple sequences and heat integrated sequences are compared to find the best structure with the minimum total annual cost.

Step 2: controllability analysis

The first step of the analysis was the selection of the controlled and manipulated variables for the investigated systems. Considering a simple two product distillation column, the column had two degrees of freedom, which might be used to specify top and bottom compositions. The distillation column was a 5 × 5 system: the controllers manipulated all five inputs (L, B, V, D and Q) in order to keep the five outputs (reflux drum level and column bottom level, pressure, top and bottom product compositions). Since the levels and pressure must be controlled at all times to ensure the stable operation, the level and pressure loops were first designed (Tamayo et al., 2008) and, in the next step, the composition control loops could be designed for the distillation column.

In the second step, the aim was to find the best controllable sequences designed and optimized in step 1. Controllability was analyzed through Morari resiliency index (MRI), condition number (CN) and relative gain array (RGA), which were frequency-dependent indices. The MRI is the smallest singular value of the open-loop transfer function. It is the poorer gain of the process (poorer sensitivity), which corresponds to specific input and output directions. The set of manipulated variables that gives the largest MRI over the frequency range of interest is preferred. Open-loop dynamic responses to step changes around the assumed operating point were obtained using the commercial software. Transfer function matrices (G) were then collected for each arrangement and they were subjected to singular value decomposition (SVD):

$$G = V\Sigma W^{\text{H}} \tag{9}$$

Table 2
Feed and product specifications.

Product	Feed		
Product groups	Components		X_i (mol fraction)
A	Propene	A: C_3H_6	0.4586
B	Propane	B: C_3H_8	0.2915
C	i-Butene	C1: C_4H_8	0.1552
	n-Butane	C2: C_4H_{10}	0.0359
D	n-Pentane	D1: C_5H_{12}	0.0419
	n-Hexane	D2: C_6H_{14}	0.0168

where $\Sigma = \text{diag}(\sigma_1, \ldots, \sigma_n)$ and σ_i = singular value of $G = \lambda 1/2(\text{GGH})$, $V = (\upsilon_1, \upsilon_2, \ldots)$ Matrix of left singular vectors and $W = (w_1, w_2, \ldots)$ matrix of right singular vectors. The most important controllability index is CN, which is derived from the singular value decomposition of transfer function. The CN is the ratio of the maximum singular value (σ^*) to the Morari resiliency index (σ^*), typically used for selecting the best set of manipulated variables:

$$\text{CN} = \frac{\sigma^*}{\sigma_*} \tag{10}$$

It provides a numerical indication of the sensitivity balance in a multivariable system. Large CNs indicate unbalanced sensitivity and also sensitivity to changes in process parameters. Therefore, sets of manipulated variables with small CNs over the frequency range of interest are preferred. RGA is a matrix that determines the interaction among control loops in a multivariable process and it is frequently used for selecting the control pairing. Each element of the RGA is defined as the ratio of the open-loop gain for a selected output when all the loops in the process are open to its open-loop gain while all the other loops are closed. Pairings that have RGA close to the unity matrix at the frequencies around the bandwidth are preferred. All MRI, CN and RGA depend on the frequency and, for this reason; they are evaluated in the frequency domain. These parameters provide a qualitative assessment of the theoretical control properties of the alternative designs. The system with higher Morari resiliency indices and lower condition numbers are expected to show the best dynamic performance under the feedback control. A full MRI analysis should cover a sufficiently complete range of frequencies. For this initial analysis of the integrated schemes to the conventional configurations, the SVD properties were simply evaluated for each separation system at zero frequency. Such analysis should give some preliminary indication of the control properties of each system around the nominal operating point. To compare the controllability of different distillation arrangements, their controllability indexes were analyzed.

3. The case study

The industrial process examined in this paper was the high temperature separation section of olefin plant which separated a multi-component flow to four categories of products with the purity of 0.98. The intake flow had the temperature of 59.39 °C and pressure of 1899.5 kPa and entered the process with the flow rate of 1355 kmol/h. Compositions of the process intake flow and groups of products are shown in Table 2. The sequence of the initial process was the distributed type, which is shown in Fig. 1A, and was regarded as a basis for comparison with other types. A number of different complex sequences were obtained with their heat integration, as shown in Figs. 1–5. The results of design and optimization are shown in Table 3. In Figs. 6–9, the MRI and CN for all possible composition control structures of all the arrangements are plotted in the frequency domain. Aspen plus simulator was used for simulation and optimization. The results of simulation export to MATLAB and controllability analysis were done in this software.

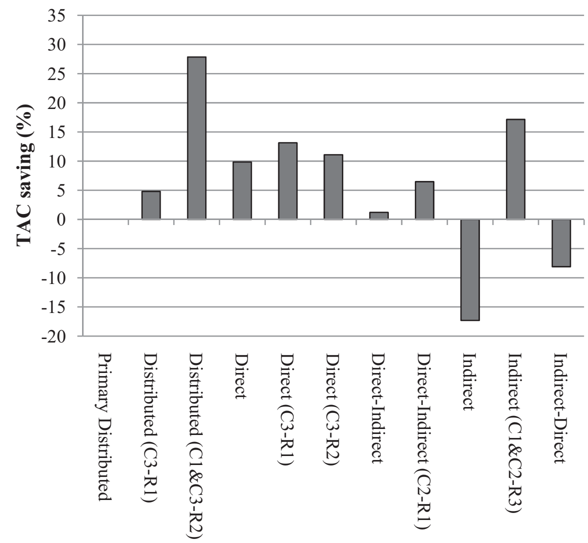

Fig. 4. Comparison of TAC saving in all sequence.

4. TAC analysis

The distributed sequence of the initial process was considered as the reference of comparison for other sequences (Fig. 1A). The optimal schemes data in Table 3 shows that the sequence distributed (C1&C3–R2) (Fig. 1C) with the TAC optimization of 27.86% represents a better result in comparison with other states. In the sequence distributed (C1&C3–R2), as can be seen in Table 3 and Fig. 1B, by increasing the pressures of columns 1 and 3 and creating the proper temperature difference, the heat output of these columns was transferred to the reboiler of column 2; thus, the cooling costs of condensers 1 and 3 were eliminated and the heating of the reboiler of column 2 was considerably reduced. This resulted in the reduction of operational costs to the amount of 27.51% compared with the reference case. In this state, the reboilers of all the columns were fed with the LP steam which lowered the cost of consumption of steam in the reboilers. Moreover, new designs of columns and heat exchangers decreased initial costs to the amount of 30.78%. At the end, TAC was decreased by 27.86%. Among the reasons involved in the high efficiency of this sequence, one was the separation of products of groups A and B in column 2 away from the products of groups C and D. The products A and B were propane and propylene. Because their relative volatilities were close to each other, their separation was difficult. Their molar percentage while entering the process was high compared it hotter compounds which caused the high heat consumption and diameter and height of column 2 to be higher than other columns in the process. One can say that, in this sequence, as a result of separating products A and B in one column and also in the intermediate columns of the process, better conditions were provided for the possibility of better heat integration and lower annual costs.

According to Table 3, sequences indirect (C1&C2–R3) (Fig. 4B) with the TAC optimization of 17.15%, direct (C3–R1) (Fig. 2B) with the optimization of 13.14%, direct (C3–R2) (Fig. 2C) with the optimization of 11.1%, direct (Fig. 2A) with the optimization of 9.85%, direct–indirect (C2–R1) (Fig. 3B) with the optimization of 6.48%, distributed (C3–R1) (Fig. 1B) with the optimization of 4.8% and direct–indirect (Fig. 3A) with the optimization of 1.2%, respectively, represented better results compared with the initial sequence. The sequences Indirect (Fig. 4A) and indirect–direct (Fig. 5) increased the TAC 17.31% and 8.11%, respectively.

Table 3
Optimal schemes.

Description	Primary distributed			Distributed (C3–R1)			Distributed (C1&C3–R2)		
	Col. 1	Col. 2	Col. 3	Col. 1	Col. 2	Col. 3	Col. 1	Col. 2	Col. 3
Pressure (kPa)	1785	1940	735	1901	2217	2748	2989	2220	1042
Diameter (m)	3.35	4.88	1.67	3.35	4.89	1.74	3.41	4.92	1.72
Reflux ratio	0.71	8.45	0.64	0.72	8.53	0.79	0.77	8.62	0.74
Actual plates	54	163	43	54	166	42	43	167	44
Heating rate (kJ/h)		111,423,972			106,272,677			78,498,124	
Cooling rate (kJ/h)		117,477,072			107,204,581			82,738,403	
HX duty (kJ/h)		–			7314222.4			32,886,838	
Steam cost ($/a)		4535992.7			4557609.8			3,326,005	
C.W cost ($/a)		1843659.3			1682445.1			1298478.3	
Operating cost ($/a)		6,379,652			6240054.9			4624483.2	
Capital cost ($/a)		758906.59			555824.96			525335.21	
TAC ($/a)		7138558.6			6795879.9			5149818.4	
Operating cost saving (%)		–			2.19			27.51	
Capital saving (%)		–			26.76			30.78	
TAC saving (%)		–			4.8			27.86	

Description	Direct			Direct (C3–R1)			Direct (C3–R2)		
	Col. 1	Col. 2	Col. 3	Col. 1	Col. 2	Col. 3	Col. 1	Col. 2	Col. 3
Pressure (kPa)	2365	2113.22	651	2414	1969	1698	2313	1839	2667
Diameter (m)	6.29	2.39	1.68	6.29	2.38	1.71	6.28	2.37	1.74
Reflux ratio	8.95	1.21	0.65	8.97	1.2	0.73	8.93	1.18	0.78
Actual plates	176	42	41	174	40	44	176	40	49
Heating rate (kJ/h)		100,110,119			94,211,676			96,031,322	
Cooling rate (kJ/h)		105,533,811			96,995,376			97,473,954	
HX duty (kJ/h)		–			7,832,094			7279755.3	
Steam cost ($/a)		4224193.8			4127335.1			4238147.6	
C.W cost ($/a)		1656224.4			1522224.1			1529734.8	
Operating cost ($/a)		5880418.2			5649559.2			5767882.4	
Capital cost ($/a)		554833.01			550778.59			578258.09	
TAC ($/a)		6435251.2			6200337.8			6346140.5	
Operating cost saving (%)		7.83			11.44			9.59	
Capital saving (%)		26.89			27.42			23.8	
TAC saving (%)		9.85			13.14			11.1	

Description	Direct–indirect			Direct–indirect (C2–R1)			Indirect		
Pressure (kPa)	2080	1307	1854	2024	2740	1717	1660	2335	2080
Diameter (m)	6.27	2.37	1.83	6.27	2.42	1.9	3.15	2.66	4.9
Reflux ratio	8.9	0.31	1	8.89	0.37	1.13	0.21	0.66	8.53
Actual plates	174	44	42	174	49	46	47	45	169
Heating rate (kJ/h)		109,826,812			96,202,845			129,266,330	
Cooling rate (kJ/h)		113,397,355			99,389,758			131,605,362	
HX duty (kJ/h)		–			14,648,275			–	
Steam cost ($/a)		4,634,066			4414348.8			5696958.1	
C.W cost ($/a)		1779633.1			1,559,801			2065385.6	
Operating cost ($/a)		6413699.2			5974149.8			7762343.7	
Capital cost ($/a)		639173.17			701488.26			611662.27	
TAC ($/a)		7052872.3			6,675,638			8,374,006	
Operating cost saving (%)		−0.53			6.36			−21.67	
Capital saving (%)		15.78			7.57			19.4	
TAC saving (%)		1.2			6.48			−17.31	

Description	Indirect (C1&C2–R3)			Indirect–direct		
	Col. 1	Col. 2	Col. 3	Col. 1	Col. 2	Col. 3
Pressure (kPa)	2585	2986	2169	1844	2296	1912
Diameter (m)	3.2	2.71	4.92	3.18	5.01	1.89
Reflux ratio	0.25	0.72	8.61	0.22	8.69	1.12
Actual plates	51	49	168	48	167	44
Heating rate (kJ/h)		82,072,805			117,517,206	
Cooling rate (kJ/h)		83,029,960			120,136,244	
HX duty (kJ/h)		48,112,352			–	
Steam cost ($/a)		4003977.4			5307057.3	
C.W cost ($/a)		1303053.9			1885391.8	
Operating cost ($/a)		5307031.3			7,192,449	
Capital cost ($/a)		607282.93			525,144	
TAC ($/a)		5914314.3			7,717,593	
Operating cost saving (%)		16.81			−12.74	
Capital saving (%)		19.98			30.8	
TAC saving (%)		17.15			−8.11	

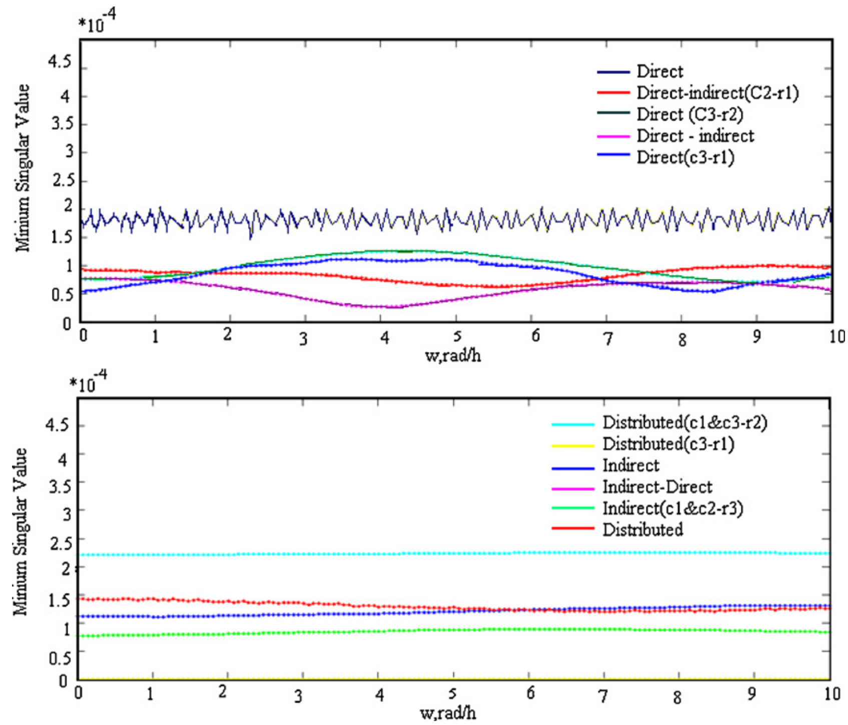

Fig. 5. Minimum singular values at low frequencies.

5. MRI and CN analysis

The MRI technique (SVD technique) requires transfer function matrices, which are generated by implementing step changes in the manipulated variables of the optimum design of the distillation sequences and registering dynamic responses of the six products. It can be mentioned that, for a system with a single input and a single output, the zeros and poles of the transfer function give important information for evaluating the full controllability of the system; however, for multivariable systems, the SVD analysis provides the theoretical control properties. For the distillation sequences presented in this work, six controlled variables were considered, i.e., the product composition A, B, C1, C2, D1, D2 (Table 2). Similarly, six manipulated variables were defined. After optimum designs were

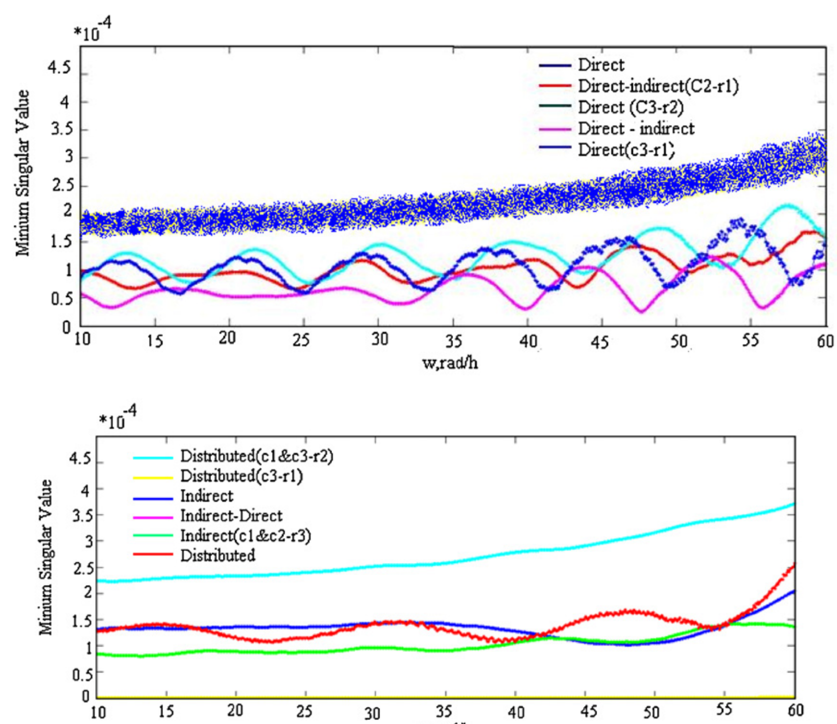

Fig. 6. Minimum singular values at intermediate frequencies.

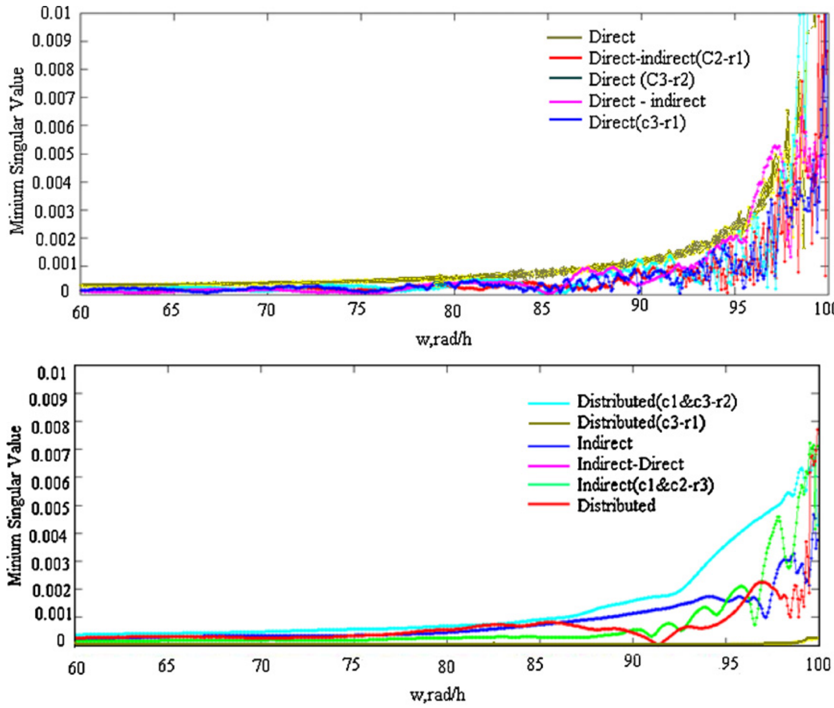

Fig. 7. Minimum singular values at high frequencies.

obtained, open-loop dynamic simulations were obtained in order to achieve the transfer function matrix. A programming language was used for formulating and finding the transfer function and demonstrating the changes of control properties to frequencies.

Figs. 5 and 6 demonstrate the Morari resiliency index at low and intermediate frequencies. In general, lower values of the condition number and higher values of the Morari resiliency index are preferred. Therefore, it can be expected that the distributed (C1&C3–R2) system exhibit better control properties than other sequences under feedback control and they are better conditioned to the effect of disturbances than other distillation schemes. Fig. 7 demonstrates the Morari resiliency index at high frequencies. Also, it shows that the distributed (C1&C3–R2) system had higher values of Morari resiliency index at high frequencies. As a result, distributed (C1&C3–R2) system had the highest singular values for the whole frequency range when compared with all arrangements.

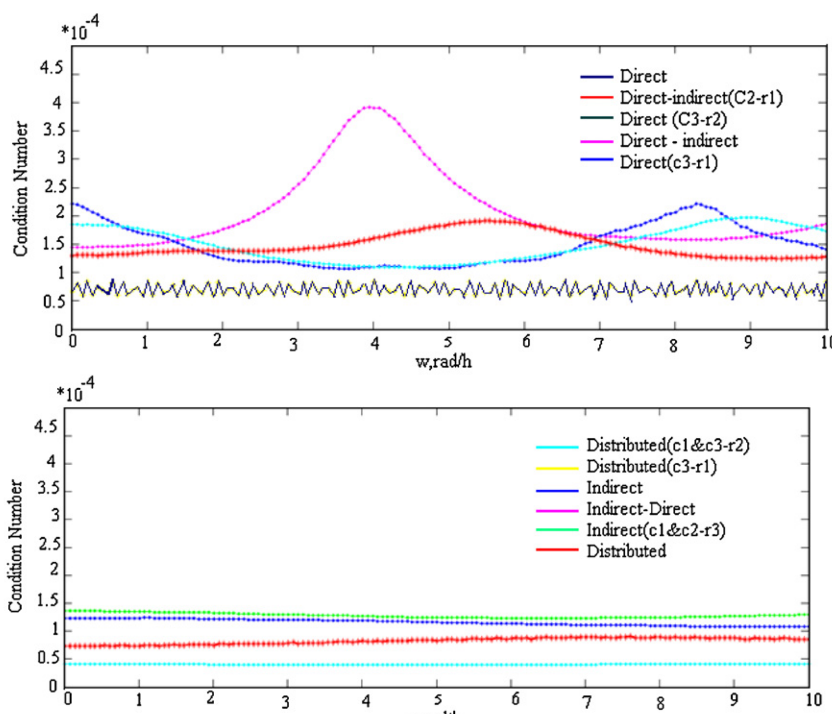

Fig. 8. Condition numbers at low frequencies.

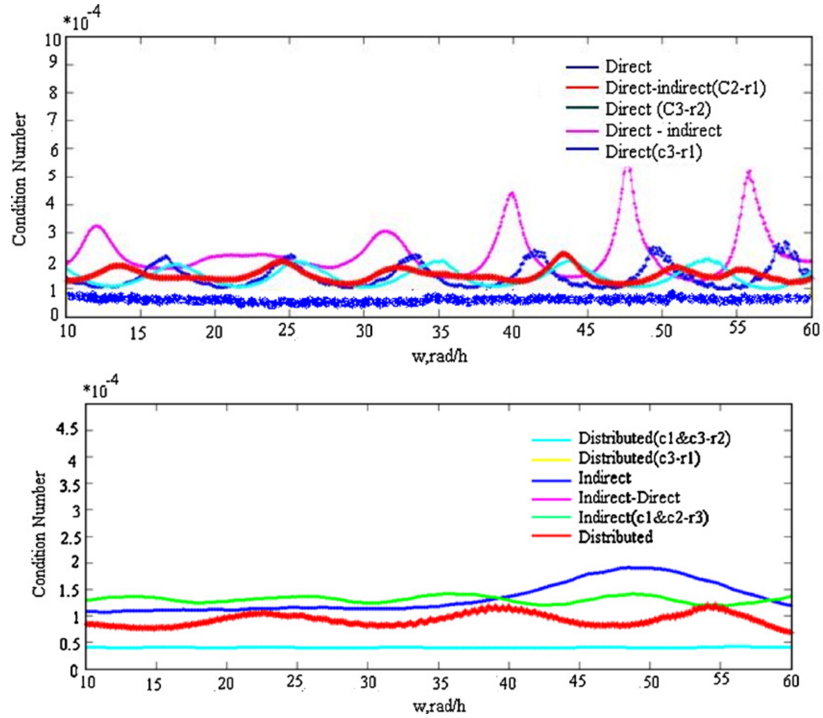

Fig. 9. Condition numbers at intermediate frequencies.

Figs. 8 and 9 demonstrate the condition numbers at low and intermediate frequencies. These two figures indicate that the distributed (C1&C3–R2) system had the lower values of the condition number. Fig. 10 demonstrates the condition numbers at high frequencies. The distributed (C1&C3–R2) system had the lower values of 17 condition numbers at high frequencies. As a result, distributed (C1&C3–R2) system had the lowest condition numbers for the whole frequency range when compared with all arrangements.

It can be seen that distributed (C1&C3–R2) system had smaller CN and higher values of Morari resiliency index at high frequencies than other structures. Therefore, according to these controllability indices, the controllability of the distributed (C1&C3–R2) system was better. Table 4 shows the ranking of sequences by TAC saving and CN and MRI analyses in the frequency domain. The MRI and CN methods showed almost the same results for the controllability of the considered sequences.

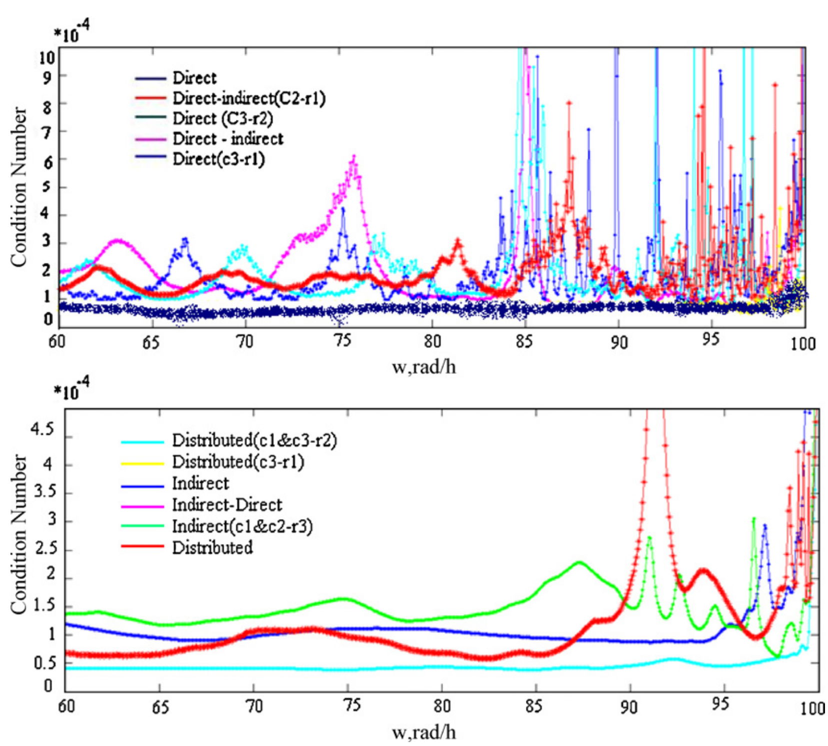

Fig. 10. Condition numbers at high frequencies.

Table 4
Ranking of sequences by TAC saving and CN and MRI analysis.

Sequences	TAC saving	CN analysis	MRI analysis
Distributed (C1&C3–R2)	1	1	1
Indirect (C1&C2–R3)	2	6	5
Direct (C3–R1)	3	10	10
Direct (C3–R2)	4	9	9
Direct	5	2	2
Direct–indirect (C2–R1)	6	7	6
Distributed (C3–R1)	7	11	11
Direct–indirect	8	4	7
Distributed	9	3	3
Indirect–direct	10	8	8
Indirect	11	5	4

6. RGA analysis

RGA was considered as the controllability index. It was also used for selecting appropriate pairings. The relative gain arrays (RGAs) were obtained for the best controllable sequence founded with SVD and CN analyses. For the distributed (C1&C3–R2) sequence, the relative gain arrays are indicated in the matrix below.

$$\Lambda = G \times (G^{-1})^T = \begin{bmatrix} 0.5746 & -0.4276 & 0.4635 & -0.3138 & 0.1728 & 0.0553 \\ 0.0813 & 1.0792 & 0.1457 & -0.6359 & -0.1458 & -0.2658 \\ 0.1506 & -0.3758 & 1.0519 & 0.0486 & 0.0511 & 0.0475 \\ -0.3263 & -0.8502 & 0.7897 & 1.2885 & -0.7855 & -0.7849 \\ -0.0281 & -0.5529 & 0.3275 & 0.3254 & 1.3256 & 0.3240 \\ -0.0984 & -0.6216 & 0.4388 & 0.4361 & 0.4353 & 1.4339 \end{bmatrix}$$

There are six controlled variables (composition A, B, C1, C2, D1, and D2) and six manipulated variables. In the RGA matrix, rows are manipulated variables and columns are controlled variables. Pairings that have RGA arrays close to the unity at frequencies around the bandwidth are preferred. According to the RGA, the pairing showing the lowest interaction for the sequence distributed (C1&C3–R2) is (RR2–x_A, BU2–x_B, RR3–x_{C1}, RR3–x_{C2}, BU3–x_{D1}, BU3–x_{D2}), where x_A is A molar purity, x_B is B molar purity, x_{C1} is C1 molar purity, x_{C2} is C2 molar purity, x_{D1} is D1 molar purity, x_{D2} is D2 molar purity, RR2 is reflux ratio of column 2, BU2 is boil up ratio of column 2, RR3 is reflux ratio of column 3 and BU3 is the boil up ratio of column 3. In the first row, it can be seen that composition A should be controlled by the manipulating reflux ratio of column 2; the second row of the relative gain array suggests that a good pairing is composition B and the boil up ratio of column 2; in the third row, the control loop for composition C1 should be made by manipulating the reflux ratio of column 3;the fourth row indicates a pairing between the composition C2 and the reflux ratio of column 3; the fifth row indicates that the composition D1 should be controlled by manipulating the boil up ratio of column 3; finally, the last row indicates that a good pairing is composition D2 and boil up ratio of column 3. It is important to note that the relative gain array of the matrix shows the diagonal control loop pairing.

7. Conclusions

Upon the analysis of the MRI, CN, and RGA in the frequency domain, the controllability of the column sequences with or without heat integration were compared for a given separation problem. According to the Morari resiliency index (MRI) and the CN analyses, the best controllable sequence was distributed (C1&C3–R2) (Fig. 1C). The MRI and CN methods showed almost the same results about the controllability of the considered sequences. The distributed (C1&C3–R2) sequence (Fig. 1C) had the maximum controllability among all the sequences meaning that this sequence had the minimum cost of control systems. RAG analysis also showed that the appropriate pairings with the lowest interaction for the distributed (C1&C3–R2) sequence was (RR2–x_A, BU2–x_B, RR3–x_{C1}, RR3–x_{C2}, BU3–x_{D1}, BU3–x_{D2}). The distributed (C1&C3–R2) sequence also had the minimum total annual cost. Thus, this sequence was the best configuration for heat integrated separation system in the considered case study. By considering all three controllability indices at the frequency range of interest, it was concluded that the distributed (C1&C3–R2) sequence had better controllability properties than other sequences. This result was very important because it indicated this sequence with lower energy requirements and the minimum of total annual cost operating at optimal operating conditions and had the best controllability of all the sequences. It proved that the heat integrated sequence with the minimum energy requirements could operate by the best controllability properties.

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