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Short communication

Control properties of thermally coupled distillation sequences for different operating conditions

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Abstract

The understanding of 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. Thermally coupled distillation sequences (TCDS) can provide significant energy savings with respect to the operation of sequences based on conventional distillation columns. TCDS exhibit a complex structure, with recycle streams, that appear to affect their controllability properties. One potential solution to this problem has been suggested through the operation of TCDS under conditions that do not provide minimum energy consumption. The basic idea is that if one changes the operation point, the control properties might change as well. In this work, we analyze the dynamic behavior of two TCDS structures under different operating points, including the one with minimum energy consumption. The control analysis properties are analyzed with the application of the singular value decomposition technique at zero frequency and closed-loop dynamic responses using standard PI controllers. The results show that the controllability properties of distillation sequences may change significantly depending on the selected operation point.

Keywords: Thermally coupled distillation schemes; Control properties; Energy consumption

1. Introduction

Certainly, the 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 overcome, secure the position of the distillation and even make it more attractive for use in the future. The main disadvantage of the distillation is its high-energy requirements. To improve the energy efficiency of separation processes based on distillation, several strategies have been proposed; one of them calls for the use of complex sequences. For example, thermal coupling has been used in the design of multicomponent distillation systems in order to reduce both energy consumption and capital costs when compared with conventional simple column configurations. TCDS for ternary mixtures have particularly been analyzed with special interest due to the remixing in the intermediate component (presented naturally in the conventional distillations sequences and associated with higher demands of energy) is reduced and the use of the energy improved (Hernández, Pereira-Pech, Jiménez, & Rico-Ramírez, 2003; Triantafyllou & Smith, 1992). There is a considerable amount of literature on the analysis of the relative advantages of TCDS for ternary separations with equilibrium (Annakou & Mizsey, 1996; Dünnebier & Pantelides, 1999; Hernández & Jiménez, 1996, 1999a; Hernández, Segovia-Hernández, & Rico-Ramírez, 2006; Tedder & Rudd, 1978; Yeomans & Grossmann, 2000 among others) and nonequilibrium (Abad-Zarate, Segovia-Hernández, Hernández, & Uribe-Ramírez, 2006) models. These studies have shown that those thermally coupled distillation schemes with side columns are capable of achieving typically 30% of energy savings compared with the conventional schemes. Two of the schemes that have received special attention are the systems with side columns: the thermally coupled system with a side rectifier (TCDS-SR, Fig. 1) and the thermally coupled system with a side stripper (TCDS-SS, Fig. 2). Also, the

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Nomenclature

FL	interconnecting liquid flow (kmol/h)
FV	interconnecting vapor flow (kmol/h)
F1	feed of composition 40/20/40 (%mol)
F2	feed of composition 15/70/15 (%mol)
G	transfer function matrix
IAE	integral of the absolute error criterion
K_c	proportional gain
M1	mixture of *n*-pentane/*n*-hexane/*n*-heptane
PI	proportional integral controller
Q	reboiler heat duty (kW)
TCDS	thermally coupled distillation sequences
TCDS-SR	thermally coupled distillation sequence with side rectifier
TCDS-SS	thermally coupled distillation sequence with side stripper

Greek symbols

γ^*	condition number
σ^*	maximum singular value
σ_*	minimum singular value
τ_I	integral time

thermally coupled distillation sequences for the separation of ternary mixtures, over a wide range of relative volatilities and feed compositions, have been reported to provide a better thermodynamic efficiency than the conventional distillation configurations (Flores, Cárdenas, Hernández, & Rico-Ramírez, 2003; Hernández-Gaona, Cárdenas, Segovia-Hernández, Hernández, & Rico-Ramírez, 2005).

The understanding of the control properties of columns with thermal couplings for the separation of ternary mixtures is an extremely important issue because many times designs with economic incentives conflict with their operational characteristics. Fidkowski and Krolikowski (1990), among others, pointed out that despite their energy savings, TCDS options may show controllability problems because of their integrated nature. For that reason, TCDS options have not been implemented extensively in the process industries until recent times (Kaibel & Schoenmakers, 2002). There have been conducted numerous research works on TCDS aiming at the dynamic performance analysis, especially for ternary mixtures (Abdul Mutalib & Smith, 1998; Hernández & Jiménez, 1999b; Jiménez, Hernández, Montoy, & Zavala-García, 2001; Segovia-Hernández, Hernández, & Jiménez, 2002a, 2002b, 2005a, 2006; Segovia-Hernández, Hernández, Jiménez, & Femat, 2005; Segovia-Hernández, Hernández, Rico-Ramírez, & Jiménez, 2004; Serra, Espuña, & Puigjaner, 1999, 2003; Serra, Perrier, Espuña, & Puigjaner, 2001; Wolff & Skogestad, 1995). Those works have found the rather unexpected result that the control properties of the integrated sequences were better than those of the conventional schemes in many cases, so that the predicted savings in both energy and capital would probably not be obtained at the expense of operational and control problems. In this work, we analyze the dynamic performance of two TCDS structures under different operating points, including the one with minimum energy consumption. The control analysis properties are analyzed with the application of the singular value decomposition technique and closed-loop dynamic responses using standard PI controllers.

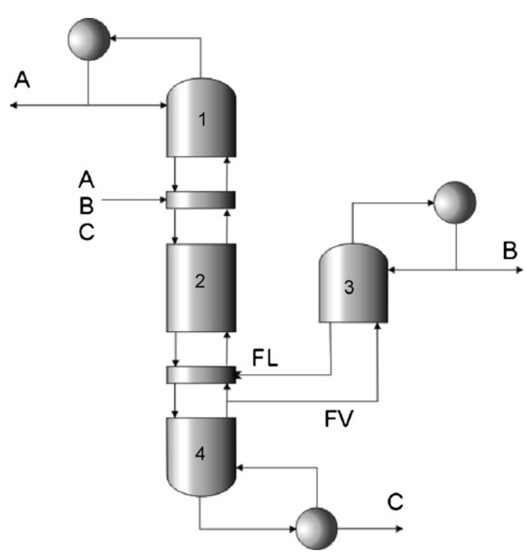

Fig. 1. Thermally coupled distillation sequences with a side rectifier (TCDS-SR).

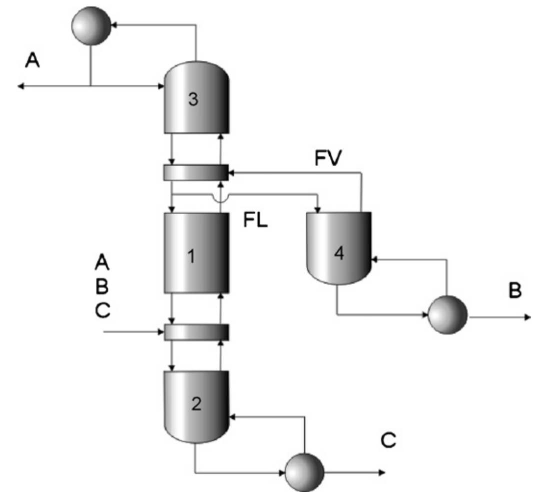

Fig. 2. Thermally coupled distillation sequences with a side stripper (TCDS-SS).

2. Design of TCDS

The design and optimization strategies for conventional distillation sequences involving the separation of ternary mixtures (Fig. 3) are well-known. The energy-efficient design methods for TCDS-SR and TCDS-SS schemes are described in Hernández and Jiménez (1996). Basically, preliminary designs of the TCDS options are obtained from the conventional sequences (Fig. 3). The design of TCDS-SR column is obtained by using a thermal link in the vapor phase in the conventional direct sequence,

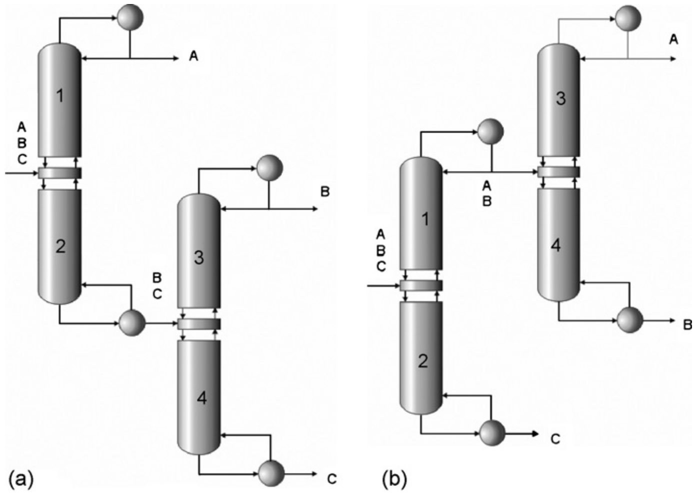

Fig. 3. Conventional distillation sequences for the separation of ternary mixtures: (a) direct sequence and (b) indirect sequence.

which eliminates the reboiler in the second column of the conventional scheme, and the tray section (named 4) is moved to the bottom of the first column of conventional scheme (Figs. 1 and 3a). The vapor flow (FV) is changed until the minimum energy demand in the reboiler of the TCDS-SR sequence is obtained. The energy-efficient design of TCDS-SS option is obtained directly from the conventional indirect distillation sequence by removing the condenser in the second column of conventional scheme and introducing a thermal coupling in the liquid phase; the tray section named 3 is moved to the top of the first column of conventional scheme (Figs. 2 and 3b). The liquid stream (FL) is varied until the minimum energy requirement for TCDS-SS column is obtained.

3. Singular value decomposition (SVD)

The understanding of 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. As the disturbance in process variables under actual operation conditions are almost inevitable, the prediction of the transient response of a distillation column bears much importance in the sense of the effective control of the separation process (Berber & Karadurmus, 1989). In this work, open loop dynamic responses to set point changes around the assumed operating point were obtained as first step. Transfer function matrices (G) were then collected for each case, and they were subjected to singular value decomposition. For more details about SVD see Klema & Laub, 1980, for example.

That mathematical operation presents three parameters of interest: the minimum singular value (σ_*) the maximum singular value (σ^*) and the ratio maximum to minimum singular values, or condition number (γ^*):

$$\gamma^* = \frac{\sigma^*}{\sigma_*} \tag{1}$$

Table 1
Mixture analyzed and feed composition

Mixture	Components (A, B, C)
M1	*n*-Pentane/*n*-hexane/*n*-heptane

Feed	Composition (%mol)
F1	40/20/40
F2	15/70/15

The condition number reflects the sensitivity of the system under uncertainties in process parameters and modeling errors. The minimum singular value is a measure of the invertibility of the system and represents a measure of the potential problems of the system under feedback control. These parameters provide a qualitative assessment of the 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 (Klema & Laub, 1980). For this initial analysis of the coupled schemes to the conventional 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 (similar analysis has been done by Hernández & Jiménez, 1999b; Segovia-Hernández, Hernández, & Jiménez, 2005; Segovia-Hernández, Hernández-Vargas, Márquez-Muñoz, Hernández, & Jiménez, 2005).

4. Cases of study

The energy savings obtained in the TCDS structure, for ternary separations, depend strongly on the amount of intermediate component. For that reason, two feed compositions were assumed for the mixture M1 (Table 1), with a low or high content of the intermediate component. The mixtures description is given in Table 1; the feed flowrate was 45.36 kmol/h as saturated liquid and the specified purities for the product streams were assumed as 98.7, 98 and 98.6% for A, B and C respectively. The design pressure for each separation was chosen to ensure the use of cooling water in the condensers. Since the feed involves a hydrocarbon mixture, the Chao–Seader correlation was used for the prediction of thermodynamic properties (Seader & Henley, 1998). It is important to establish that studying a three-component mixture of hydrocarbons is a suitable example, given the applications of the hydrocarbon mixtures in the petrochemical industry (Harmsen, 2004). The tray arrangements and some parameters for the TCDS-SR and TCDS-SS after optimization task for the case of study M1F1 is given in Tables 2 and 3.

5. Results

Two sets of analysis were carried out: (i) the theoretical control properties of thermally coupled distillation sequences were obtained using SVD technique and (ii) *servo-control*: step was induced as set point changes for each product composition under SISO feedback control at each output flowrate. Both set of

Table 2
Design variables for the TCDS-SS (M1F1)

	Main column	Side stripper
Pressure (atm)	1.44	1.44
Stages	29	8
Feed stage	20	
Interconnection stage	10	
FL (kmol/h)	25.3	

Table 3
Design variables for the TCDS-SR (M1F1)

	Main column	Side rectifier
Pressure (atm)	1.43	1.43
Stages	36	10
Feed stage	9	
Interconnection stage	17	
FV (kmol/h)	37.2	

simulations were analyzed in the optimal operation conditions (optimal reboiler duty) and nonoptimal operation conditions obtained by fixing FL or FV (depending of the arrangement) in different values (remembering that reboiler duty is function of the FL or FV values).

5.1. SVD analysis

The 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 the dynamic responses of the three products. In this work, the reflux flowrate, and the reboiler heat duty were chosen as the manipulated variables. Serra et al. (1999) have explained that working out of the optimal operating conditions, the controllability of the dividing wall column may improve. Thus, it will be interesting to compare the controllability of the TCDS with side column at nonoptimal conditions.

For the TCDS-SR and TCDS-SS several operational conditions are analyzed: the optimal operation (FL or FV are used to optimize the reboiler duty) and five nonoptimal operation values. Logically, nonoptimal values have a higher reboiler duty than the optimal operation. The reboiler duty and FL or FV values are indicated in Tables 4–7. To compare the controllability of the different operation values, their controllability indexes are analyzed (minimum singular value and condition number). In the Tables 4–7, the σ_* and γ^* for all cases of study are showed.

There are important differences between the column operated at optimal operation and the column operated at nonoptimal condition. In the case of TCDS-SR (M1F1), when it is operated at nonoptimal conditions (FV = 31.7 kmol/h; see Table 4) its controllability improves. In those nonoptimal conditions, TCDS-SR present highest value of the minimum singular value (Table 4); therefore, it can be expected that coupled system exhibit better control properties than the sequence, in optimal condition, under feedback control. The results for the condition number show that sequence in the nonoptimal value offer the best value (Table 4). As a result, it can be expected that thermally coupled distillation system in a different operating condition is better conditioned to the effect of disturbances than the optimal arrangement. As has been explained, the operation in nonoptimal conditions has a higher energy consumption than optimal conditions. Consequently when the reboiler duty is increased, the controllability has improved. The reboiler duty is lower than the conventional sequence (Table 13) in the case when the controllability parameters are better than the optimal scheme. Similar results are showed for TCDS-SR (M1F2) in the Table 5.

Table 4
Reboiler duty, minimum singular value and condition number for TCDS-SR (M1F1)

FV (kmol/h)	Q (kW)	σ_*	γ^*
24.9	1506.6	25.8	67.3
28.1	1056.4	28.4	53.4
31.7	832.6	29.3	48.5
35.4	756.2	27.4	79.2
37.2 (optimal value)	746.9	26.6	80.9
40.8	762.7	25.6	81.3

Table 5
Reboiler duty, minimum singular value and condition number for TCDS-SR (M1F2)

FV (kmol/h)	Q (kW)	σ_*	γ^*
61.2	2494.1	0.2	18645.3
66.2	1302.9	0.5	12285
68.0	1174.6	3.1	1984.1
72.6	1059.1	1.8	3057.4
76.6 (optimal value)	1042.7	0.7	4020.6
80.7	1052.0	0.1	19736.2

Table 6
Reboiler duty, minimum singular value and condition number for TCDS-SS (M1F1)

FL (kmol/h)	Q (kW)	σ_*	γ^*
18.1	1131.8	65.9	14.7
19.4	912.9	80.4	12.2
20.4	805.8	99.1	10.6
22.6	668.8	55.2	16.7
25.3 (optimal value)	636.9	49.9	18.5
29.5	656.2	42.2	22.3

Table 7
Reboiler duty, minimum singular value and condition number for TCDS-SS (M1F2)

FL (kmol/h)	Q (kW)	σ_*	γ^*
49.9	2753.4	1.7	2483.0
53.7	1249.8	3.7	1983.2
56.7	988.7	4.4	558.8
62.6	894.3	4.0	788.2
64.2 (optimal value)	893.4	3.5	1040.7
72.5	925.9	2.1	2328.1

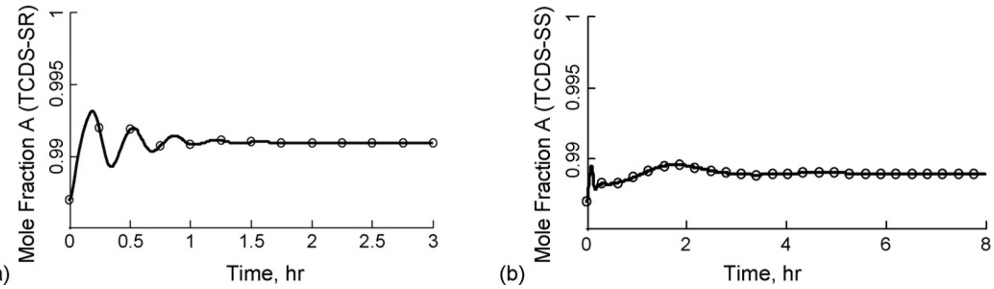

Fig. 4. Closed loop dynamic response for component A (M1F1) in the optimal reboiler duty: (a) TCDS-SR and TCDS-SS.

In the Table 6, the energy consumption and the $\sigma*$ and γ^* for the TCDS-SS (M1F1) are showed. When the arrangement operated at optimal conditions is compared, it can be seen that the TCDS-SS has the lower energy consumption. However, the optimal arrangement has bad control properties. In the case of nonoptimal conditions (FL = 20.4 kmol/h; see Table 6) the scheme has better control properties. The nonoptimal complex schemes show higher values of the minimum singular value and offer the best values in the condition number. Therefore, it can be expected that that these coupled systems exhibit better control properties than the optimal sequences under feedback control and it can be expected that system are better conditioned to the effect of disturbances than the optimal arrangements. Those are very important results that show how, taking advantage of the complexity offered by the TCDS, a convenient operation point (not necessarily the optimal condition) with low energy consumption and good controllability can be chosen. Similar results are showed for TCDS-SS (M1F2) in the Table 7. One more time, the reboiler duty is lower than the conventional sequence (Table 13) in the case when the controllability parameters are better than the optimal scheme.

5.2. Dynamic simulations

The closed loop analysis was based on proportional-integral (PI) controllers. Several alternatives exist for tuning up the controller parameters. We attempted a common ground for comparison by optimizing the controller parameters, proportional gains (K_c) and integral times (τ_I), for each conventional and integrated scheme following the integral of the absolute error (IAE) criterion. For the integrated arrangements, the procedure is particularly complicated because of the interactions of the multivariable control problem. For these cases, the tuning procedure was conducted taking one control loop at a time. Thus, the parameters obtained were taken from the following control loop until the three loops were considered. Those tuning parameters are presented in Table 8 (case M1F1). For the dynamic analysis, individual set point changes for product composition were implemented for each of the three product streams (as showed in Figs. 4–6). The liquid compositions for the main product streams A, B and C were taken as the controlled variables whereas, respectively, the reflux flowrate and the reboiler heat duty were chosen as the manipulated variables. For all cases (optimal and

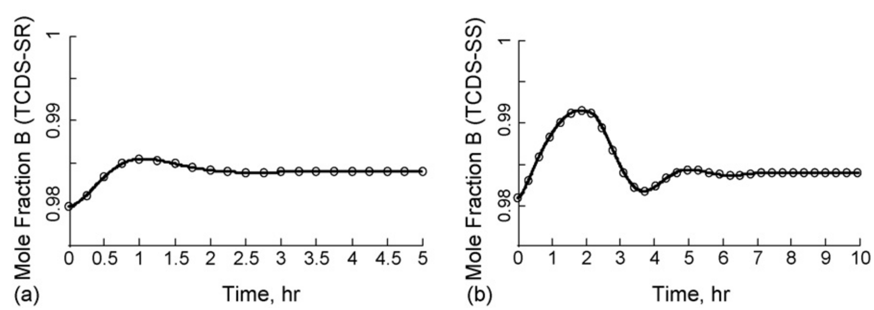

Fig. 5. Closed loop dynamic response for component B (M1F1) in the optimal reboiler duty: (a) TCDS-SR and TCDS-SS.

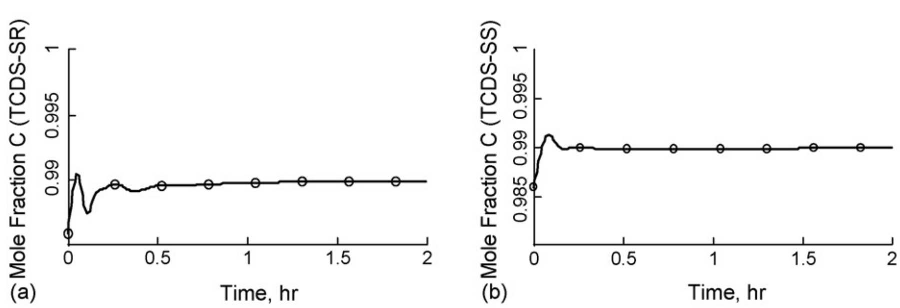

Fig. 6. Closed loop dynamic response for component C (M1F1) in the optimal reboiler duty: (a) TCDS-SR and TCDS-SS.

Table 8
Tuning parameters obtained for each control loop (case M1F1)

Control loop	TCDS-SR	TCDS-SS
A		
Gain	450 kmol/kmol	480 kmol/kmol
Integral time	0.2 h	0.3 h
B		
Gain	12 kmol/kmol	550 kW
Integral time	160 h	1.1 h
C		
Gain	500 kW	390 kW
Integral time	0.1 h	0.1 h

nonoptimal conditions), the three control loops were assumed to operate under closed loop fashion. The performance of the sequences under analysis was compared through the evaluation of IAE values for each test. This part of the study was conducted with the use of Aspen Dynamics 11.1.

Table 9 shows the IAE values obtained for each composition control loop of the six cases for mixture M1, when feed F1 was considered. The TCDS-SR offered the best dynamic behavior, based on the lowest values of IAE, for the control of the three product streams in the value of FV = 31.7 kmol/h. This result is similar at the case analyzed by SVD. The best values of minimum singular value and condition number was for the same FV value. This situation corroborates that operating in nonoptimal conditions is a good option. In the case of TCDS-SR (M1F2) the best values of IAE are obtained in FV = 68 kmol/h (see Table 10). The control of the lightest component (A), intermediate (B) and heaviest component (C) does not create any significant problems in that nonoptimal operation point. This best FV value get is equal to that obtained with SVD technique.

Table 9
IAE results for TCDS-SR (M1F1)

FV (kmol/h)	Component	IAE
24.9	A	3.4780E−05
	B	2.141E−04
	C	6.3500E−06
28.1	A	2.1993E−05
	B	1.8700E−04
	C	5.0100E−06
31.7	A	1.3030E−05
	B	1.1400E−04
	C	4.2470E−06
35.4	A	4.6000E−05
	B	7.5700E−04
	C	5.3400E−06
37.2 (optimal value)	A	4.8736E−05
	B	1.8192E−03
	C	5.4422E−06
40.8	A	5.1600E−05
	B	3.6840E−03
	C	5.5810E−06

Table 10
IAE results for TCDS-SR (M1F2)

FV (kmol/h)	Component	IAE
61.2	A	3.3813E−05
	B	9.0250E−05
	C	4.7100E−06
66.2	A	2.2994E−05
	B	6.8100E−05
	C	4.4700E−06
68.0	A	1.5296E−05
	B	1.5033E−05
	C	4.0700E−06
72.6	A	3.9300E−05
	B	5.3380E−04
	C	4.2887E−06
76.6 (optimal value)	A	4.1049E−05
	B	1.0800E−03
	C	4.3057E−06
80.7	A	4.3600E−05
	B	1.5870E−03
	C	4.4041E−06

The analysis was completed with the consideration of the TCDS-SS. In Table 11 are displayed the IAE results for the case M1F1. The best nonoptimal value of FL is 20.4 kmol/h. This result is equal to that obtained with SVD analysis for this case. If the control policy calls for the change of set point composition of the three components, the TCDS-SS, in nonoptimal value, shows the best behavior, with the lowest value of IAE and the reboiler duty is lower than the conventional sequence (Table 11). The case of TCDS-SS (M1F2) is analyzed in the Table 12. The value of FL = 56.7 kmol/h is the best option. In this value the

Table 11
IAE results for TCDS-SS (M1F1)

FL (lbmol/h)	Component	IAE
18.1	A	2.7472E−05
	B	3.4400E−05
	C	5.9866E−06
19.4	A	1.0075E−05
	B	3.2518E−05
	C	3.0560E−06
20.4	A	2.2230E−06
	B	3.2165E−05
	C	2.4552E−06
22.6	A	2.5182E−05
	B	3.3300E−05
	C	6.9370E−06
25.3 (optimal value)	A	3.0143E−05
	B	5.3643E−05
	C	7.3955E−06
29.5	A	3.1012E−05
	B	2.6570E−03
	C	7.5617E−06

Table 12
IAE results for TCDS-SS (M1F2)

FL (lbmol/h)	Component	IAE
49.9	A	1.9640E−05
	B	1.4632E−05
	C	4.3206E−06
53.7	A	1.8967E−05
	B	1.2935E−05
	C	2.3270E−06
56.7	A	1.0878E−05
	B	1.1878E−05
	C	1.9460E−06
62.6	A	2.2354E−05
	B	1.6969E−05
	C	5.4350E−06
64.2 (optimal value)	A	2.2605E−05
	B	2.8032E−05
	C	5.4990E−06
72.5	A	2.3212E−05
	B	6.4620E−04
	C	5.8302E−06

Table 13
Energy requirements (kW) for the separation of the ternary mixtures using conventional sequences

Feed	Direct sequence	Indirect sequence
F1	956.5	1039.5
F2	1228.0	1276.7

coupled scheme offered the best dynamic behavior, based on the lowest values of IAE, for the control of the three product streams. This result is consistent with the values obtained using singular value decomposition (Table 13)

6. Conclusions

Upon analysis of the SVD and dynamic simulations, the controllability of TCDS-SR and TCDS-SS in different operating conditions are compared for a given separation problem. Through an optimization procedure, the reboiler duty of the complex arrangements is minimized. At optimal operation, the TCDS controllability is worse than the controllability in nonoptimal conditions (not minimized reboiler duty). However, the TCDS operating at nonoptimal conditions, their controllability is much better. In the case of nonoptimal condition the energy consumption is higher that the arrangement in optimal conditions. In the best nonoptimal case, the reboiler duty is lower that the conventional sequence. The results obtained using SVD are similar to the results obtained using rigorous dynamic simulations. In general, the result is very important because it indicates that TCDS with side column operated at some nonoptimal operating conditions have the best controllability and the lower energy consumption.

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