DYNAMIC ANALYSIS OF DISTILLATION WITH THERMAL COUPLING FOR DIFFERENT OPERATING CONDITIONS

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Thermally coupled distillation sequences (TCDS) exhibit a more complex structure, with recycle streams, that appear to affect their controllability properties. One potential solution to this problem is considering 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 performance of two TCDS structures (in particular, systems with side columns) 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. The results show that the controllability properties of distillation sequences may change significantly depending on the selected operation point. In particular, we show that the dynamic properties of TCDS can be improved by switching from a design with minimum energy consumption to another one in which a higher level of energy consumption is allowed (but an energy consumption lower than the conventional schemes).

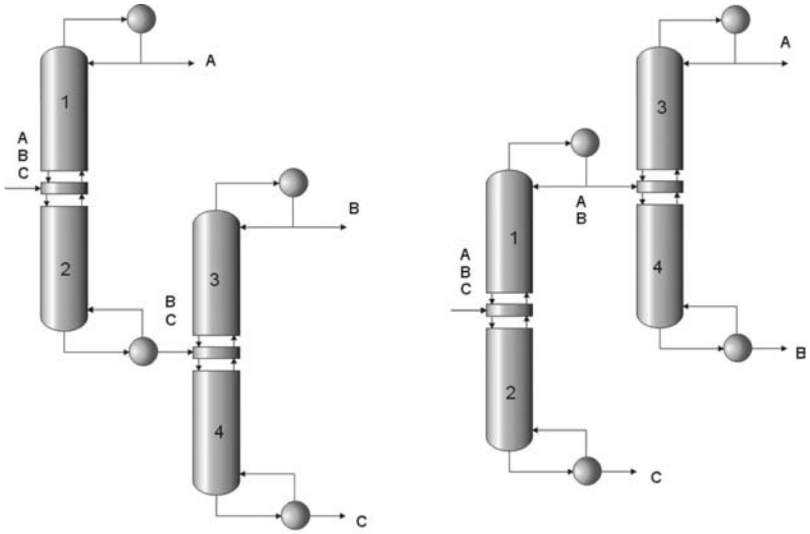
KEYWORDS: Control properties, thermally coupled distillation sequences.

INTRODUCTION

It is well known that conventional distillation sequences consume large amounts of energy in the reboilers; as a result, researchers are interested in developing distillation schemes that can reduce both energy requirements and capital costs. An interesting alternative is the implementation of thermally coupled distillation sequences (TCDS). Such separation sequences have proved to lower energy consumption around 30% in comparison to conventional distillation trains for the separation of ternary mixtures (Tedder and Rudd, 1978; Triantafyllou and Smith, 1992; Hernández and Jiménez, 1996). It has been explained in the works of Triantafyllou and Smith (1992) and Hernández et al. (2003) that the TCDS options can reduce the energy consumption because they do not have remixing, in contrast to conventional distillation sequences. Remixing can be explained if one considers the separation of a ternary mixture (A, B, C) by using a conventional direct distillation sequence. In the first column of the direct distillation sequence, component A is obtained as overheads and components B and C are obtained as bottom products, which are separated in the next column. If the composition profile of the intermediate component B in the liquid phase of the first column is analyzed, the composition of component B increases below the feed stage until a maximum is reached and then the composition decreases. This is known as remixing and is associated with higher energy consumption because, in order to repurify the mixture, additional energy will be required in the next column. Energy savings are obtained with the introduction of optimal values of the flow rates of the recycle streams. Also, the introduction of a vapor or a liquid recycle stream eliminates a reboiler or a condenser respectively. The understanding of the control properties of columns with thermal couplings for the separation of ternary mixtures, is an issue of extreme importance since many times designs with economic incentives conflict with their operational characteristics. In particular, the presence of recycle streams for TCDS schemes has influenced the notion that control problems might be expected during the operation of those systems with respect to the rather well-known behavior of conventional distillation sequences. For that reason, TCDS options have not been implemented extensively in the process industries until recent times (Kaibel and Shoenmakers, 2002). In many works, about TCDS for ternary mixture, some authors (Wolff and Skogestad, 1995; Abdul-Mutalib and Smith, 1998; Segovia – Hernández et al., 2002a; Segovia – Hernández et al., 2002b; Serra et al., 2003; Segovia – Hernández et al., 2004; Segovia – Hernández et al., 2005a; Segovia – Hernández et al., 2005b) 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.

ENERGY – EFFICIENT DESIGNS

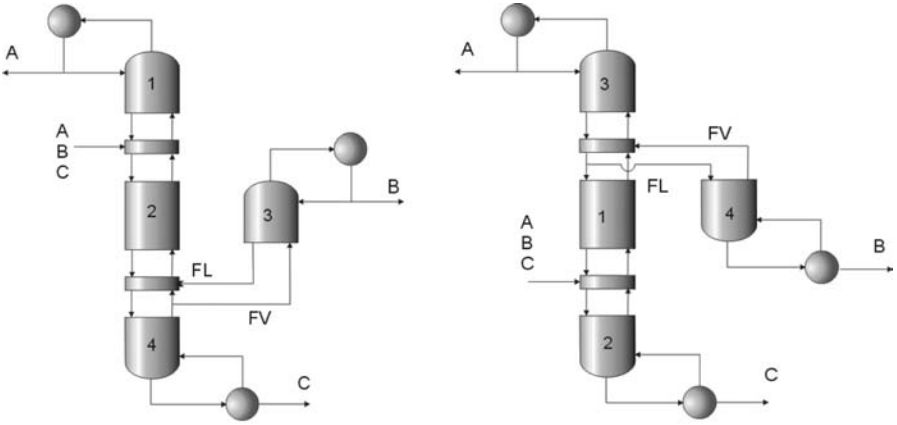
The design and optimization strategies for conventional distillation sequences involving the separation of ternary mixtures (Figure 1) are well–know. The energy – efficient design methods for the thermally coupled system with a side rectifier (TCDS-SR, Figure 2a) and the thermally coupled system with a side stripper (TCDS-SS, Figure 2b) schemes are described in Hernández and Jiménez (1996). Basically, preliminary designs of the TCDS options are obtained from the conventional sequences (Figure 1). The design of TCDS – SR column is obtained by using a thermal link in the vapor phase in the conventional direct 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 (Figure 1a and 2a). 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



a) Direct Sequence (DS)

b) Indirect Sequence (IS)

Figure 1. Conventional distillation sequences for the separation of ternary mixtures



a) TCDS - SR

b) TCDS - SS

Figure 2. Thermally coupled distillation sequences for the separation of ternary mixtures

phase; the tray section named 3 is moved to the top of the first column of conventional scheme (Figure 1b and 2b). The liquid stream (FL) is varied until the minimum energy requirement for TCDS – SS column is obtained.

SINGULAR VALUE DECOMPOSITION (SVD)

Open loop dynamic responses to set point changes around the assumed operating point (which corresponds to that with minimum energy consumption for each configuration) were obtained. The responses were obtained through the use of Aspen Dynamics. Transfer function matrices (G) were then collected for each case, and they were subjected to SVD:

$$G = V\Sigma W^{H} \tag{1}$$

where $\Sigma = \mathrm{diag}\ (\sigma_1, \ldots, \sigma_n)$, σ_i = singular value of $G = \lambda_i^{\frac{1}{2}}\ (GG^{H})$; $V = (v_1, v_2, \ldots)$ matrix of left singular vectors, and $W = (w_1, w_2, \ldots)$ matrix of right singular vectors. Two parameters of interest are the minimum singular value, σ^*, and the ratio maximum to minimum singular values, or condition number:

$$\gamma^{*} = \sigma^{*}/\sigma* \tag{2}$$

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. The condition number reflects the sensitivity of the system under uncertainties in process parameters and modeling errors. 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 (Lau et al). A full SVD analysis should cover a sufficiently complete range of frequencies. For this initial analysis of the alternative schemes to the coupled 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.

CASE OF STUDY

It is well know that 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 each mixture [F1, (40/20/40); F2, (15/70/15); % mole], with a low or high content of the intermediate component. The mixtures is n-pentane / n-hexane / n-heptane; the feed flowrate was 45.36 kmol/hr. 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. 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).

RESULTS

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

SVD ANALYSIS

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 2– 5. To compare the controllability of the different operation values, their controllability indexes are analyzed (minimum singular value and condition number). In the Tables 1–2, the $\sigma*$ and γ^* for the cases of study M1F1 are showed. There are important differences between the column operated at optimal operation and the column operated at non-optimal condition. In the case of TCDS – SR (M1F1), when it is operated at nonoptimal conditions (FV = 31.7 kmol/hr; see Table 2) its controllability improves. In those nonoptimal conditions, TCDS – SR present highest value of the minimum singular value (Table 1). Therefore, it can be expected that coupled system exhibit better control properties than the optimal sequences under feedback control and that they are better conditioned to the effect of disturbances than the optimal arrangements. The results for the condition number show that the sequence in the nonoptimal value offer the best value (Table 1). As a

Table 1. Reboiler duty, minimum singular value and condition number for TCDS – SR (M1F1)

FV (kmol/hr)	Q (kW)	$\sigma*$	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 2. Reboiler duty, minimum singular value and condition number for TCDS – SS (M1F1)

FL (kmol/hr)	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

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, operation in nonoptimal conditions has a higher energy consumption than optimal conditions. Consequently when the reboiler duty is increased, the controllability has improved. Similar results are showed for TCDS – SR (M1 F2). In the Table 2, 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 see 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/hr; see Table 2) 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 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. This is a very important result 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 (M1 F2).

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 reset 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; the parameters thus obtained were taken for the following control loop until the three loops were considered. For the dynamic analysis, individual set point changes for product

Table 3. IAE results for TCDS − SR (M1F1)

FV (kmol/hr)	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

composition were implemented for each of the three product streams. For all cases (optimal and 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 3 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/hr. This result is similar to the case analyzed by SVD. The best values of minimum singular value and condition number were for the same FV value. This situation corroborate that operate in nonoptimal conditions is a good option. Similar results were obtained in all cases of study.

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 a 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 indicate that TCDS with side column operated at some nonoptimal operating conditions has the best controllability and the lower energy consumption.

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REFERENCES

Abdul-Mutalib, M.I., and Smith, R. 1998. Operation and Control of Dividing Wall Distillation Columns. Part I: Degrees of Freedom and Dynamic Simulation, *Trans Inst. Chem. Eng.*, 76, 308.

Harmsen, G.J., 2004, Industrial Best Practices of Conceptual Process Design, *Chem. Eng. Processes*, 43, 671.

Hernández, S., and Jiménez, A., 1996, Design of Optimal Thermally - Coupled Distillation Systems Using a Dynamic Model, *Trans IChemE*, 74, 357.

Hernández, S., Pereira-Pech, S., Jiménez, A., and Rico-Ramírez, V., 2003, Energy Efficiency of an Indirect Thermally Coupled Distillation Sequence. *The Can. J. Chem. Eng.*, 2003; 81 (5) 1087.

Kaibel, G., and Schoenmakers, H., 2002, Process Synthesis and Design in Industrial Practice, In *Proceedings of ESCAPE - 12 (Computer Aided Process Engineering, 10)*, Grievink, J., Schijndel, J. V., Eds.; Elsevier; Amsterdam, The Netherlands.

Lau, H., Álvarez, J., and Jensen, K.F., Synthesis of Control Structures by Singular Value Analysis, *AIChE J*, 31, 427.

Segovia - Hernández, J.G., Hernández, S., and Jiménez, A., 2002a, Control Behaviour of Thermally Coupled Distillation Sequences, *Trans Inst. Chem. Eng.*, 80, 783.

Segovia - Hernández, J.G., Hernández, S., Jiménez, A., 2002b, Análisis Dinámico de Secuencias de Destilación Térmicamente Acopladas, *Información Tecnológica*, 13 (2) 103.

Segovia - Hernández, J.G., Hernández, S., Rico – Ramírez, V., and Jiménez, A., 2004, A Comparison of the Feedback Control Behavior between Thermally Coupled and Conventional Distillation Schemes, *Comput. Chem. Eng.*, 28, 811.

Segovia - Hernández, J.G., Hernández, S., and Jiménez, A., 2005a, Analysis of Dynamic Properties of Alternative Sequences to the Petlyuk Column, *Comput. Chem. Eng.*, 29, 1389.

Segovia - Hernández, J.G., Hernández, S., Jiménez, A., Femat, R., 2005b, Dynamic Behavoir and Control of the Petlyuk Scheme Via a Proportional – Integral Controller with Disturbance Estimation, *Chem. Biochem. Eng. Q. J.*, 19 (3), 243.

Serra, M., Espuña, A., and Puigjaner, L., 2003, Controllability of Different Multicomponent Distillation Arrangements, *Ind. Eng. Chem. Res.*, 42, 1773.

Tedder, D. W., and Rudd, D. F., 1978, Parametric Studies in Industrial Distillation: Part I. Design Comparisons, *AIChE J*, 24, 303.

Triantafyllou, C., and Smith, R., 1992, The Design and Optimization of Fully Thermally Coupled Distillation Columns, *Trans Inst. Chem. Eng.*, 70, 118.

Wolff, E. A., and Skogestad, S., 1995. Operation of Integrated Three – Product (Petlyuk) Distillation Columns, *Ind. Eng. Chem. Res.*, 34, 2094.