CONTROL PROPERTIES OF ALTERNATIVE SCHEMES TO THERMALLY COUPLED DISTILLATION COLUMNS FOR TERNARY MIXTURES SEPARATIONS

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The thermally coupled distillation schemes have received considerable attention because of their efficiency to reduce the energy required for the separation of multicomponent mixtures. The structure of the complex systems offers some control challenges arising from the transfer of vapor (or liquid) streams between the columns. Recently, some alternate schemes to thermally coupled distillation arrangements for the separation of ternary mixtures, that might provide better operational properties than the complex columns, have been proposed. In this work, we analyze the control properties of two alternative distillation schemes to the coupled systems. The theoretical control properties have been analyzed with the application of the singular value decomposition technique. The results indicate that a reduction in the number of interconnections of the alternate configurations does not necessarily provide an improvement of their control properties.

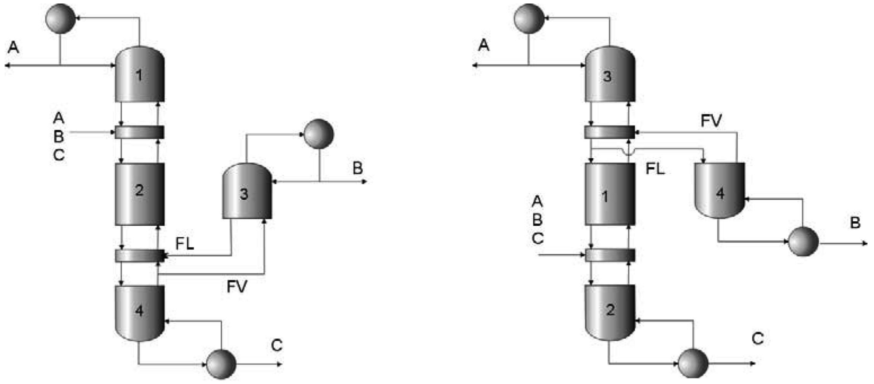
KEYWORDS: thermally coupled distillation sequences, alternatives schemes, control properties

INTRODUCTION

The main disadvantage of the distillation is its high - energy requirements. Several techniques are used to overcome this problem like integration of the distillation column with the overall process which can give significant energy savings (Smith and Linnhoff, 1998) but this kind of improvement can be limited. Significant energy savings can be reached by the use of complex distillation arrangements such as thermally coupled distillation sequences (TCDS). In the case of the TCDS, through the implementation of a vapor-liquid interconnection between two columns, a condenser or a reboiler of one of the columns is eliminated, and if a proper search on the operating conditions is performed, such an interconnection can provide energy savings (Hernández and Jiménez, 1996; Hernández and Jiménez, 1999). 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, Figure 1a) and the thermally coupled system with a side stripper (TCDS-SS, Figure 1b). Theoretical studies (Tedder and Rudd, 1978; Annakou and Mizsey, 1996; Dünnebier and Pantelides, 1999; among others) have shown that these thermally coupled distillation schemes with side columns are capable of achieving typically 30% of energy savings compared with the conventional schemes. 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. Fidkowski and Krolikowski (1990), among others, pointed out that despite their energy savings, TCDS options may show controllability problems because of their integrated nature. 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, some authors (Wolff and Skogestad, 1995; Abdul-Mutalib and Smith, 1998; Jiménez *et al.*, 2001; Segovia-Hernández *et al.*, 2002) 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. Recently, Agrawal (2000) have reported some alternate configurations to TCDS schemes for the separation of ternary mixtures, eliminated the recycle streams, that appear to have some operational advantages over expected dynamic properties of the designs of TCDS-SR and TCDS-SS. In this work we analyze the control properties of two alternative distillation schemes to the coupled systems and compare them to the original configuration.

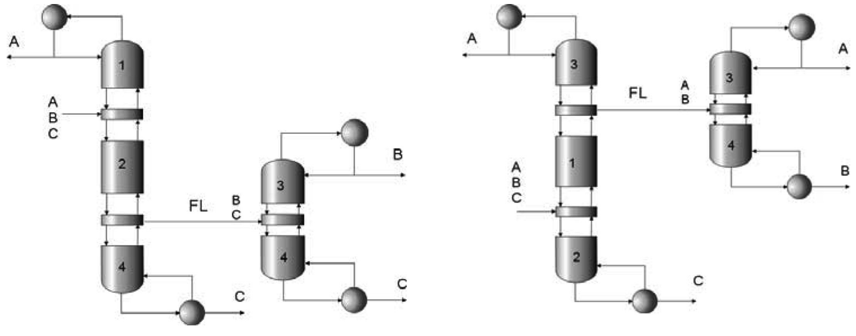
ALTERNATIVE SCHEMES TO TCDS WITH SIDE COLUMNS

Agrawal (2000) has proposed two arrangements that emerge from modifications to the systems shown in Figure 1. Such new systems are shown in Figures 2. The alternate



a) TCDS - SR b) TCDS - SS

Figure 1. Thermally coupled distillation sequences for the separation of ternary mixtures



a) ATCDS - SR

b) ATCDS - SS

Figure 2. Alternate arrangement to the TCDS for the separation of ternary mixtures

arrangement to TCDS-SR, a direct sequence with a side stream from the first column (ATCDS-SR, Figure 2a) eliminates the recycle stream of the TCDS-SR sequence by reproducing the bottom section (section 4; see Figure 2a) of the first column within the second column, which affects the structure of the original side rectifier. In the other case, the alternative arrangement to TCDS-SS, an indirect sequence with a side stream from the first column (ATCDS-SS, Figure 2b), the vapor interconnection of the TCDS-SS scheme is eliminated and the top section of the first column (section 3; see Figure 2b) is added to the second column, affecting the original side stripper. Therefore, the new arrangements do not contain recycle streams, and the second column of each sequence is transformed into a conventional distillation column. The resulting new structures, therefore, seem to provide simpler systems to control and operate.

ENERGY – EFFICIENT DESIGNS

The design of the two TCDS under consideration was carried out following the procedure suggested by Hernández and Jiménez (1996). The method provides a tray structure for the integrated systems by a section analogy procedure with respect to the design of a conventional sequence; the TCDS-SR is obtained from the tray arrangements of a direct sequence and the TCDS-SS from an indirect sequence. The degrees of freedom that remain after design specifications (one degree of freedom for the systems with side columns) were used to obtain the operating conditions under which the integrated designs provide minimum energy consumption. The search procedure provided the optimal values of the interconnecting vapor flowrate (FV) for the TCDS-SR (Figure 1a) or the interconnecting liquid flowrate (FL) for the TCDS-SS (Figure 1b). Rigorous simulations, using the dynamic model developed by Hernández and Jiménez (1996), were conducted to test the designs. The model is based on the total mass balance, component mass balances, equilibrium relationships, summation constraints, energy balance and stage hydraulics.

Because of the coupling between the columns, the set of equations must be solved simultaneously. The new schemes were then obtained directly from the TCDS arrangements following the simple tray section analogies depicted in Figures 1–2. The new systems were also subjected to an optimization procedure to detect the values of the side stream flowrates from the first column that minimized their energy consumptions. It should be noted that the range for the search procedure for these structures is more restricted than for the TCDS structures because of mass balance considerations. Those bounds for columns with side streams have been explained by Glinos and Malone (1985). For more details to optimization method of alternative sequences, see Ramírez and Jiménez, 2004.

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:

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

where $\Sigma = \mathrm{diag}\ (\sigma_1, \ldots, \sigma_n)$, σ_i = singular value of $G = \lambda_i^{1/2}\ (\mathrm{GG^H})$; $\mathrm{V} = (\mathrm{v}_1, \mathrm{v}_2, \ldots)$ matrix of left singular vectors, and $\mathrm{W} = (\mathrm{w}_1, \mathrm{w}_2, \ldots)$ 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. 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

To compare the behavior of the sequences three ternary mixtures with different values of the ease of separability index ($\mathrm{ESI} = \alpha_{\mathrm{AB}}/\alpha_{\mathrm{BC}}$), as defined by Tedder and

Rudd (1978), were considered. The selected mixtures were n-pentane, n-hexane and n-heptane (M1, ESI = 1.04), n-butane, isopentane and n-pentane (M2, ESI = 1.86), and isobutane, n-butane and n-hexane (M3, ESI = 0.18). To examine the effect of the content of the intermediate component, two types of feed compositions were assumed. One feed with a low content of the intermediate component (where mole fractions of A, B, C, were equal to 0.40, 0.20, 0.40, feed F1) and another one with a high content of the intermediate component (A, B, C equal to 0.15, 0.70, 0.15, feed F2), were used. The total feed flowrate for all cases was 45.5 kmol/h. Specified product purities of 98.7, 98 and 98.6 percent for A, B and C respectively were assumed. The pressure operation was chosen to guarantee the use of cooling water to condenser the light component (A).

RESULTS

Tables 1–3 give the results for the SVD test for each sequence. The thermally coupled distillation systems, TCDS – SR and TCDS - SS, have the lowest value of the condition number, which implies that these sequence are better conditioned to the effect of disturbances than the alternate arrangements; such sequences also show the highest value of the minimum singular value, which means that the coupled columns are expected to require lower control efforts under feedback operation than the other alternate sequences. On the other hand, the modified structures show the worst values of the SVD parameters, which implies that, from the set of structures, these sequences are worst conditioned to the effect of disturbances.

Since the new structures were conceived to improve the control properties of the thermally coupled distillation sequences, it should be highlighted that the complex configurations do not show the worst control properties of the four sequences. The SVD parameters indicate that the theoretical properties of the modified structures (ATCDS-SR

Table 1. Minimum singular value and condition number for each structure (mixture M1)

Scheme	σ_*	γ^*
Feed F1		
TCDS-SR	29.3	80.9
ATCDS-SR	0.063	16356.24
TCDS-SS	80.4	12.2
ATCDS-SS	0.1	29392
Feed F2		
TCDS-SR	1.8	1984
ATCDS-SR	0.6	3231.5
TCDS-SS	1.7	2483
ATCDS-SS	0.0006	181674

Table 2. Minimum singular value and condition number for each structure (mixture M2)

Scheme	σ_*	γ^*
Feed F1		
TCDS-SR	41.4	125.8
ATCDS-SR	0.1	8166.1
TCDS-SS	120.8	8.9
ATCDS-SS	0.1	98594
Feed F2		
TCDS-SR	4.4	851.9
ATCDS-SR	2	1603.2
TCDS-SS	7.5	1328.8
ATCDS-SS	0.0018	273873.7

and ATCDS-SS), obtained through the elimination of one interconnecting stream, are expected to be worse than those of the original complex arrangements. Moreover, one can also notice that the reduction of one interconnection from the coupled arrangements deteriorate the theoretical controllability properties of the complex structures. The best compromise on the theoretical controllability properties provided by the SVD application seems to be provided by the thermally coupled structures. Overall, the results from this test indicate that the reduction in the number of interconnections that provides simpler designs does not necessarily drive the expected operational advantages with respect to

Table 3. Minimum singular value and condition number for each structure (mixture M3)

Scheme	σ_*	γ^*
Feed F1		
TCDS-SR	21.7	85.8
ATCDS-SR	1.7	4064.2
TCDS-SS	257.5	34.57
ATCDS-SS	0.04	10315.63
Feed F2		
TCDS-SR	5.8	977.8
ATCDS-SR	0.1	69816
TCDS-SS	3	1401.3
ATCDS-SS	0.02	17057

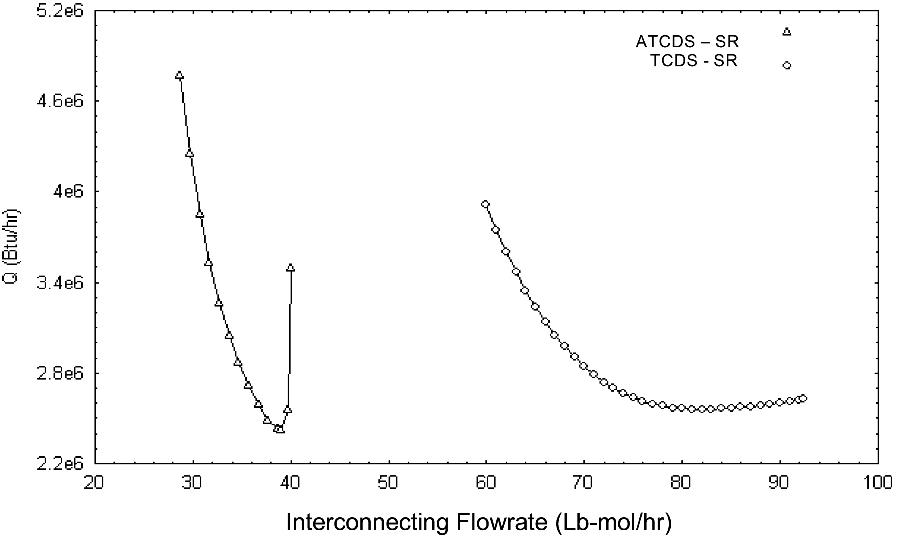


Figure 3. Search for the optimal energy consumptions for the TCDS-SR and ATCDS-SR options

the original complex configurations. There is, however, one additional issue worth discussing. The optimization curves for each type of arrangement show interesting features. Figure 3, for instance, shows the response curves obtained during the optimization for energy consumption of the TCDS-SR and the ATCDS-SR options for mixture M1, F1. Although the energy efficiency of the new structure is similar to the TCDS, the response surfaces of the TCDS-SR structure show smoother behavior than those of the new sequence. That means that variations in operating conditions will more noticeably affect the new design, which implies that such a design will very likely be more difficult to control. This observation is consistent with the results obtained using the SVD. Similar results were obtained in all cases of study. These results seem to indicate that, contrary to the original expectation, the new systems might be more difficult to control than the integrated arrangements.

CONCLUSIONS

It has been shown that the new systems can perform the separations tasks with energy efficiencies that are similar to or better than those of thermally coupled systems (see Ramírez and Jiménez, 2004). These results are important because they let conclude that the ATCDS-SR and ATCDS-SS are thermodynamically equivalent schemes to TCDS-SR and TCDS-SS respectively. Given the simpler structure, the new systems were conceived as more operable options to the integrated schemes. However, the results obtained for the response curves of each type of system show that the new designs are more sensitive to changes around the optimal operating point. The results from the theoretical control properties, evaluated from the singular value decomposition method, indicate that a reduction in the number of interconnections does not necessarily provide the operational advantages originally expected given the resulting, simpler, structural design. One major conclusion can be addressed from this initial study on control properties: the properties of the complex arrangements can be deteriorated by the reduction in the number of interconnections.

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