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CONTROL PROPERTIES ANALYSIS OF ALTERNATE SCHEMES TO THERMALLY COUPLED DISTILLATION SCHEMES

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Abstract: Recently, on the assumption that the presence of the recycle stream in thermally coupled distillation schemes (TCDS) might origin a difficult operation, some alternate arrangements that might provide better operational properties have been proposed. In this work, on the framework of singular value analysis, control properties of two alternate schemes were assessed and compared with their corresponding TCDS. The results show that the alternate schemes, in which the recycle streams are removed, do not necessarily provide an improvement on the control properties.

Keywords: control properties, thermally coupled distillation, singular value analysis.

1. INTRODUCTION

In a plant where distillation sequences are used to separate fluid mixtures, undoubtedly there is a large amount of energy consume. Several approaches are used to overcome this problem, among them complex distillation column arrangement design with or without thermal coupling. Because of the promising savings in both energy and capital cost, a considerable amount of literature on the analysis of the relative advantages of the thermally coupled distillation schemes (TCDS) has been come into view, showing energy savings of up to 30% in comparison to the conventional distillation sequences (i. e., Tedder and Rudd, 1978; Glinos and Malone, 1988; Carlberg and Westerberg, 1989; Yeomans and Grossman, 2000; Rev, *et al.*, 2001; Rong and Kraslawski, 2003; Calzon-McConville, *et al.*, 2006).

Despite the potential benefits of TCDS and some reports of successful industrial applications (Kaibel and Schoenmakers, 2002) only a limited number of such columns has been implemented in the field. The lack of widespread use of TCDS can partly be attributed to their more difficult control properties (Agrawal and Fidkowski, 1998). In particular, the presence of recycle streams has influenced the notion that control problems might be expected during the operation of those systems with respect to the rather well-known behaviour of conventional distillation sequences.

The understanding of control properties of TCDS is an essential research issue since many times designs with economic incentives conflict with their operational characteristics. Then, recent publications report progress in the identification of suitable control variables/schemes for these type of complex distillation schemes (Hernández and Jiménez, 1999; Jiménez, *et al.*, 2001; Serra, *et al.*, 2003; Segovia-Hernández, *et al.*, 2004).

Focus on ternary mixtures, Agrawal (2000) reported some alternate arrangements to TCDS (Figure 1 - 2). In these novel arrangements (Figure 3 - 4) the recycle stream that appears to have some operational disadvantage in TCDS is eliminated. Since a better understanding on operation or control characteristics is required for the TCDS above mentioned, in this work an analysis on their theoretical control properties was conducted. Specifically, on the framework of the singular value decomposition (SVD) technique (Lau, *et al.*, 1985), for each scheme its sensitivity to model errors and disturbances, and its control effort were assessed through the condition number and the minimum singular value, respectively, of the corresponding transfer matrix in the frequency domain.

2. DISTILLATION ARRANGEMENTS

For ternary mixtures there are two proposed (typical) TCDS. A first scheme is created thermally coupling a first column to a rectifier (TCDS-SR) (Figure 1) by a recycle stream (vapour flowing from column to rectifier and liquid flowing back from the rectifier to the first column). The second scheme is created thermally coupling a first column to a stripper (TCDS-SS) (Figure 2) by a recycle stream (liquid flowing from the first column to the stripper and vapour flowing back from the stripper to the first column). The recycle stream in both schemes gives rise to a design and operation challenge. Agrawal (2000) addressed this problem and proposed some modifications to the TCDS that might improve its dynamics properties: eliminating the recycle streams. The first modified arrangement (SDI) (Figure 3), on the basis of the TCDS-SR, is a direct sequence with a side stream from the first column; in this arrangement the vapour interconnection is eliminated by reproducing the bottom section of the first column within the second column, affecting the structure of the original side rectifier. The second modification (SIS) (Figure 4), on the basis of the TCDS-SS, is an indirect sequence with a side stream from the first column; in this, the vapour interconnection is eliminated and the top section of the first column is added to the second column, affecting the original side stripper. Therefore, the new arrangements eliminate the intercolumn vapour transfer and do not contain recycle streams, and the second column of each scheme is transformed into a conventional distillation column.

The resulting new structures, SDI and SIS, are thermodynamically equivalent to the TCDS-SR and TCDS-SS, respectively, in the sense that they exhibit similar energy consumption and thermodynamic efficiencies (Segovia-Hernández, *et al.*, 2005c); but the new schemes seem to provide simpler systems to control and operate in comparison with the original TCDS.

3. CASES OF STUDY

To compare the behaviour of the sequences three mixtures with different values of ease of separability index (ESI) (Tedder and Rudd, 1978) were considered: (M1) n-pentane / n-hexane / n-heptane (ESI = 1.04); (M2) n-butane / i-pentane / n-pentane (ESI = 1.86); and (M3) i-pentane / n-pentane / n-hexane (ESI = 0.47). The energy savings obtained in the TCDS for ternary separations depend strongly on the amount of intermediate component; for that reason two feed compositions (% mole) were considered for each mixture: (F1) 40 / 20 / 40, and (F2) 15 / 70 / 15. F1 has a low content of the intermediate component, and F2 has a high one.

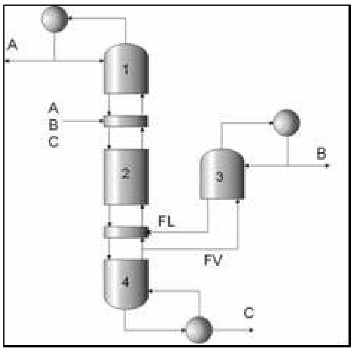

Figure 1. Thermally coupled distillation scheme with side rectifier (TCDS-SR).

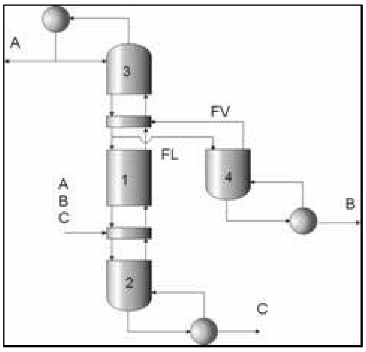

Figure 2. Thermally coupled distillation scheme with side stripper (TCDS-SS).

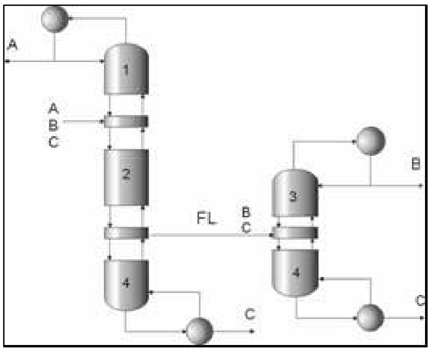

Figure 3. Modified arrangement to the TCDS-SR (SDI).

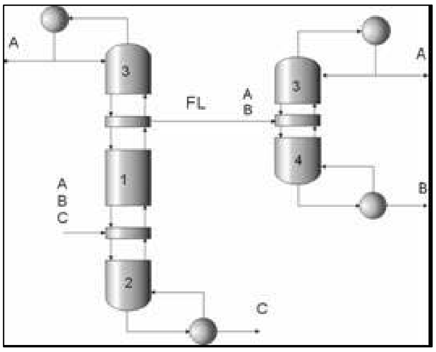

Figure 4. Modified arrangement to the TCDS-SS (SIS).

4. DESIGN METHOD

The energy-efficient design of the distillation arrangements is briefly described. For TCDS-SR and TCDS-SS design, the method proposed by Hernández and Jiménez (1996) was followed; the columns of the conventional sequence that provide the tray structure for the TCDS were designed assuming reflux ratios of 1.33 times the minimum values; and the design pressure for each separation was chosen to ensure the use of cooling water in the condensers. The alternate schemes were obtained directly from the TCDS following the simple tray section analogies depicted in Figures 1 - 4. The new systems were subjected to an optimization procedure to determine the values of the side stream flowrate from the first column that minimized their energy consumptions. It should be noted that the range for the search procedure for the new arrangements is more restricted than for the TCDS due to mass balance considerations. Those bounds for columns with side streams have been explained by Glinos and Malone (1985), and further details on the design and optimization procedure of the alternate sequences are given by Ramírez and Jiménez (2004).

5. CONTROL PROPERTIES ANALYSIS

5.1 Transfer Function Matrices

The complex distillation sequences are nonlinear and were modeled in Aspen Dynamics^{TM}, but in order to apply the SVD technique, transfer function matrices are required for each scheme-mixture-composition case, once optimum distillation design is obtained. The transfer function matrix (G(s)) is generated by identification of linear responses of outputs (control variables) originated by implementing step changes in inputs (manipulated variables).

For the TCDS three outputs were considered: the product composition (X_A, X_B, X_C). The inputs were selected according to the arrangement structure: the reflux ratios (R1 and R2), and the heat duty supplied to the reboiler (Q1) for the TCDS-SR; and the reflux ratio (R1), and the heat duties supplied to the reboiler (Q1 and Q2) for the TCDS-SS.

For the alternate arrangements, according to the arrangement structure, four outputs as well related to the product composition were considered: X_A, X_B, X_{C1}, X_{C2} for SDI, and X_{A1}, X_{A2}, X_B, X_C for SIS. One more is added due to one component is obtained in two streams. In connection, four inputs were considered: the reflux ratios (R1 and R2), and the heat duties supplied to the reboilers (Q1 and Q2).

5.2 Singular Value Decomposition (SVD)

The obtained transfer function matrices (G) were subjected to SVD in the frequency domain (Lau, *et al.*, 1985):

$$G(j\omega) = V(j\omega)\, \Sigma(j\omega)\, W^H(j\omega)$$

where Σ is the diagonal matrix whose entries are the singular values of G. From these singular values two parameters are recalled: the minimum singular value (σ_*), and the condition number ($\gamma = \sigma^*/\sigma_*$); σ^* is the maximum singular value.

The interpretation given to these parameters is recalled: a system with high γ is sensitive to modeling errors and disturbances, and a system with low σ_* potentially exhibit difficulties when implementing feedback control. Then, systems with higher σ_* and lower γ are expected to show the best dynamic performances under feedback control. It is important to note that singular values depend on the units of the variables; as a result, the scaling of the gains is necessary. In this work, the controlled variables (mole fractions) are bounded between 0 and 1 and the changes in the manipulated variables were associated to the fraction in the opening of the control valve.

6. RESULTS

In order to illustrate the obtained results, the transfer function matrices for the distillation arrangements are given for the case of mixture M1 with composition F1 (M1-F1) in the following figures:

$$\begin{array}{cc}
 & \begin{array}{ccc} \mathbf{R1} & \mathbf{R2} & \mathbf{Q1} \end{array} \\
\begin{array}{c} \mathbf{X_A} \\ \mathbf{X_B} \\ \mathbf{X_C} \end{array} &
\begin{bmatrix}
\frac{0.0072}{1+0.6325s}-\frac{0.0172}{1+5.3972s} & \frac{0.0076}{1+0.6325s}-\frac{0.0172}{1+4.09s} & -\frac{3.1976}{1+0.6325s}+\frac{3.3316}{1+2.2596s} \\
\frac{0.0204}{1+3.6731s} & \frac{0.0208}{1+3.7515s} & \frac{0.5396}{1+0.0903s}-\frac{8.046}{1+3.0539s} \\
-\frac{0.0176}{1+3.3085s} & -\frac{0.0176}{1+3.3224s} & \frac{3.3336}{1+1.4245s}
\end{bmatrix}
\end{array}$$

Figure 5. Transfer function matrix for TCDS-SR (M1-F1).

$$\begin{array}{cc}
 & \begin{array}{ccc} \mathbf{R1} & \mathbf{Q2} & \mathbf{Q1} \end{array} \\
\begin{array}{c} \mathbf{X_A} \\ \mathbf{X_B} \\ \mathbf{X_C} \end{array} &
\begin{bmatrix}
\frac{0.0144}{1+0.758s} & -\frac{1.0408}{1+0.849s} & -\frac{4.0988}{(1+0.3881s)^2} \\
-\frac{0.0028}{1+0.483s}+\frac{0.0084}{1+6.24s} & \frac{1.3644}{1+1.6786s} & \frac{0.102}{1+0.2s}-\frac{0.7592}{0.36s^2+0.72s+1} \\
-\frac{0.0128}{1+2.0659s} & -\frac{0.9688}{(1+1.1485s)^2} & \frac{1.0988}{0.2025s^2+0.54s+1}
\end{bmatrix}
\end{array}$$

Figure 6. Transfer function matrix for TCDS-SS (M1-F1).

$$\begin{array}{cc}
 & \begin{array}{cccc} \mathbf{R1} & \mathbf{R2} & \mathbf{Q1} & \mathbf{Q2} \end{array} \\
\begin{array}{c} \mathbf{X_A} \\ \mathbf{X_B} \\ \mathbf{X_{C1}} \\ \mathbf{X_{C2}} \end{array} &
\begin{bmatrix}
\frac{0.01e^{-0.05s}}{1+1.7776s} & \frac{0.0104e^{-0.05s}}{1+2.1516s} & -\frac{2.9992}{1+0.6461s} & \frac{0.0104e^{-0.05s}}{1+2.2366s} \\
\frac{0.004}{1+0.7s}-\frac{0.0028}{1+1.6s} & \frac{0.004e^{-0.07s}}{1+0.75s}-\frac{0.0028}{1+2.1s} & \frac{1.572}{1+0.16s}-\frac{3.792}{1+1.8s} & -\frac{2.5708}{1.0946s^2+2.467s+1} \\
-\frac{0.0008e^{-0.27s}}{1+0.316s}+\frac{0.002}{1+4.545s} & -\frac{0.0008e^{-0.27s}}{1+0.5s}+\frac{0.002}{1+4.585s} & \frac{0.768}{1+0.136s}-\frac{0.4252}{1+0.237s} & -\frac{0.0008e^{-0.27s}}{1+038s}+\frac{0.002}{1+5.1s} \\
\frac{0.006}{1+0.45s} & \frac{0.006}{1+0.18s} & \frac{2.9024}{1+1.1379s} & \frac{2.5908}{1+1.2157s}
\end{bmatrix}
\end{array}$$

Figure 7. Transfer function matrix for SDI (M1-F1).

$$\begin{array}{cc}
 & \begin{array}{cccc} \mathbf{R1} & \mathbf{Q1} & \mathbf{Q2} & \mathbf{R2} \end{array} \\
\begin{array}{c} \mathbf{X_{A1}} \\ \mathbf{X_B} \\ \mathbf{X_C} \\ \mathbf{X_{A2}} \end{array} &
\begin{bmatrix}
\frac{0.0068}{1+0.58s} & -\frac{1.8208}{1+0.4325s} & \frac{0.0068}{1+0.4325s} & \frac{0.0064}{1+0.4582s} \\
-\frac{0.0152e^{-0.09s}}{1+1.1s}+\frac{0.01}{1+2.8s} & \frac{0.6224}{1+0.1162s}-\frac{4.6532}{1+1.974s} & \frac{1.1616}{1+0.623s} & -\frac{0.0152e^{-0.09s}}{1+1.1s}+\frac{0.01}{1+2.8s} \\
-\frac{0.0216}{1+1.9932s} & \frac{1.8784}{1+0.8506s} & -\frac{0.0204}{1+1.7208s} & -\frac{0.0228}{1+3.0401s} \\
\frac{0.0428}{1+1.6074s} & -\frac{10.4832}{0.4904s^2+1.4807s+1} & -\frac{3.5908}{0.2799s^2+1.0999s+1} & \frac{0.0436}{1+1.9172s}
\end{bmatrix}
\end{array}$$

Figure 8. Transfer function matrix for SIS (M1-F1).

Similar matrices were obtained for the rest of the mixture-composition cases (M1-F2, M2-F1, M2-F2, M3-F1, and M3-F2); because of space restriction they are not shown.

Corresponding to the above given transfer function matrices, Figures 9 - 12 illustrates, on a log-log plot, the resulting γ and σ_* as a function of frequency. For all the arrangements, γ is above $1\text{x}10^4$; and σ_* is around $1\text{x}10^{-3}$ at low frequencies; and the control properties deteriorate at higher frequencies. Although these values indicate that all of these arrangements are sensitive to model errors and disturbances, and that considerable control effort has to be used, all of these arrangements exhibit input-output stability. Notice that all of the transfer function matrices are proper, and correspond to dynamic responses adjusted to first or parallel processes. Despite the values on control properties are not satisfying towards control design, remind that the purpose of this work is a comparison of control properties between original and alternate TCDS.

Comparing the control properties of SDI with the ones of TCDS-SR, for the case M1-F1 (Figures 9 and 10) SDI arrangement present higher values of σ_* and lower values of γ for the whole frequency range; therefore, it can be expected that SDI system exhibit better control properties, and is better conditioned to the effect of disturbances than TCDS-SR. For the case of M2-F1, at low frequencies TCDS-SR exhibit higher values of σ_*, but as the frequency increases, the σ_* decreases drastically, and the SDI offers better values of this parameter; on the other hand TCDS-SR shows the lowest values of γ at low frequencies. In general, we can say that TCDS-SR offers better conditioning properties against model uncertainties and process disturbances at low frequencies. In the case M3-F1, SDI has the highest values of σ_* and the lowest values of γ for the whole frequency range. Therefore, the SDI is better conditioned to effect of disturbances. Similar results were obtained for the other cases of study (M1-F2, M2-F2, and M3-F2). In general, it can be said that the SDI presents better control properties than the TCDS-SR; subsequently, a reduction in the number of interconnections of the alternate configuration provide an improvement of its controllability properties.

For the case of study for TCDS-SS and SIS with M1-F1 (Figures 11 and 12), TCDS-SS presents higher values of σ_* and lower values of γ for the whole frequency range. Therefore, the TCDS-SS is expected to require less effort control under feedback operation and it is better conditioned to the effect of disturbances than SIS. In the case of M2-F1, the TCDS-SS shows the better control properties than the SIS. In the case of M3-F1, the TCDS-SS seems to provide the best choice because it has the highest values of σ_* and the lowest γ at low frequencies. Similar results were obtained for the other cases of study (M1-F2, M2-F2, and M3-F2). In general, it can be said that the TCDS-SS presents better control properties than the SIS; subsequently, a reduction in the number of interconnections of the alternate configurations does not necessarily provide an improvement of its controllability properties.

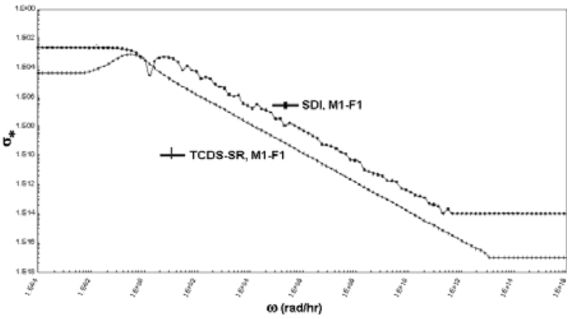

Figure 9. Minimum singular values for TCDS-SR and SDI with M1-F1.

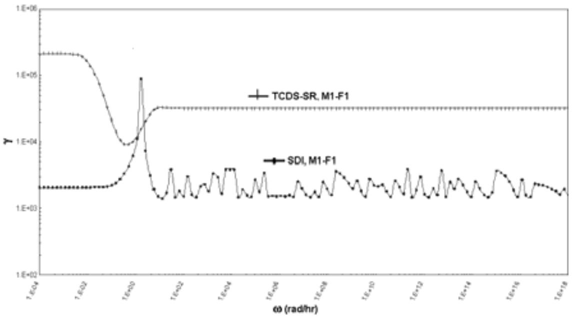

Figure 10. Condition number values for TCDS-SR and SDI with M1-F1.

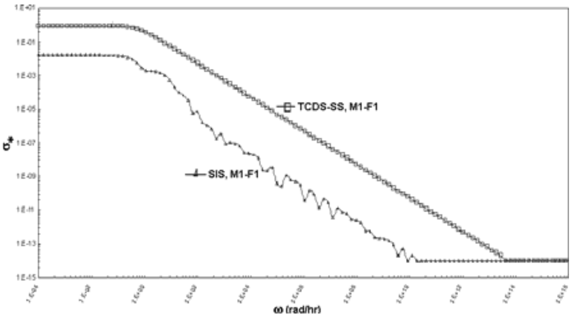

Figure 11. Minimum singular values for TCDS-SS and SIS with M1-F1.

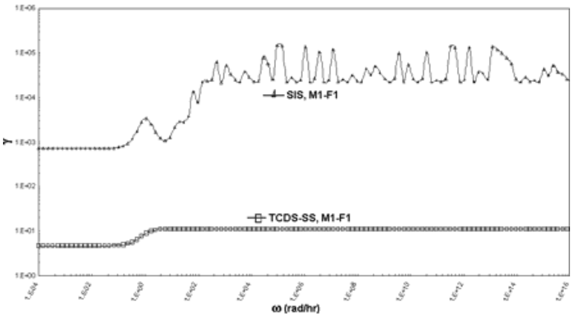

Figure 12. Condition number values for TCDS-SS and SIS with M1-F1.

Based on the observed trends, a distinction is given between the best control option for TCDS-SR and TCDS-SS with their alternate schemes, respectively. In the case of TCDS-SR and SDI, the alternate structure has better control properties; for TCDS-SS and SIS options, the original arrangement is expected to require less control efforts under feedback operation. A remark on structures can be established; when intermediate component is obtained as distillate product (TCDS-SR or SDI) the better structure is the alternate arrangement; when the intermediate component is obtained as bottoms product (TCDS-SS or SIS) the better structure is without reduction in the number of interconnections.

7. CONCLUSIONS

A comparative study on the theoretical control properties of two distillation arrangements that arise from modifications to TCDS with side columns has been conducted. Results from SVD indicate, in general, that SDI system is better than the TCDS-SR, and TCDS-SS is better than SIS scheme; and this suggests that a reduction in the number of interconnections does not necessarily give the operational advantages originally expected provided the resulting simpler structural design. This is important because one can say that the recycle streams can attenuate the effect of the disturbances.

On the other hand, the results also suggest that control properties are ruled by the position where the intermediate component is obtained in the arrangement (top or bottom): when the intermediate component is obtained as distillate product (TCDS-SR or SDI) the better structure is with reduction in the number of interconnections. When the intermediate component is obtained as bottoms product (TCDS-SS or SIS) the better structure is without reduction in the number of connections. In general, it is apparent that the presence of recycle streams instead of deteriorating the dynamic behavior of distillation arrangements, may contribute positively to their dynamic properties. This situation depends on structure and the position where the intermediate component is obtained in the arrangement.

On the understood that these results are preliminary, validation by means of a closed-loop operation analysis has to be done.

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