CONTROL PROPERTIES OF THERMALLY COUPLED EXTRACTIVE DISTILLATION SEQUENCES

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ABSTRACT

The structure of the thermally coupled distillation systems offers some control challenges arising from the transfer of vapor (or liquid) streams between the columns. In particular, the presence of recycle streams for coupled 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. In this work, we analyze the control properties of thermally coupled extractive distillation schemes. The control properties are analyzed with the application of the singular value decomposition technique and a closed-loop analysis. The results showed that the energy savings predicted in the complex extractive distillation sequence can be achieved along with good dynamic behavior and reductions in greenhouse gas emissions.

Keywords: Extractive distillation, thermally coupled systems, energy savings, dynamic behavior.

1. INTRODUCTION

The separation of azeotropic mixtures or close boiling components is a challenging task in many chemical processes due to it is impossible using a single conventional distillation column. Therefore, many nonconventional distillation techniques have been proposed to solve this problem (Doherty and Malone, 2001). The most common alternatives involve changing the operating pressure or adding a so-called entrainer compound. In both cases an additional component, the so-called entrainer, is introduced into the original mixture to facilitate a separation. Because of the easier separation of the entrainer through liquid–liquid splitting in a decanter, heterogeneous azeotropic distillation is often preferred over homogeneous azeotropic distillation. Extractive distillation is commonly applied in industry, and is becoming an important separation method in petrochemical engineering. In the classical extractive distillation setup (DS; Figure 1), the entrainer is fed into the extractive column above the process feed with the azeotrope forming components. One of these azeotrope forming components is withdrawn at the top of the extractive column, while the other, together with the entrainer, forms the bottoms product of the extractive column. In a second column, the entrainer is separated from the second feed component and recycled to the first column. The separation in the second column is easier when a large boiling point difference

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between the high-boiling entrainer and the second feed component exists and no additional azeotropes occur in the mixture. Contrary to the conventional distillation process, the dynamic of the extractive columns has been little explored in the published literature, although some authors have addressed this problem: Arifin and Chien (2008) and Luyben (2008), for example.

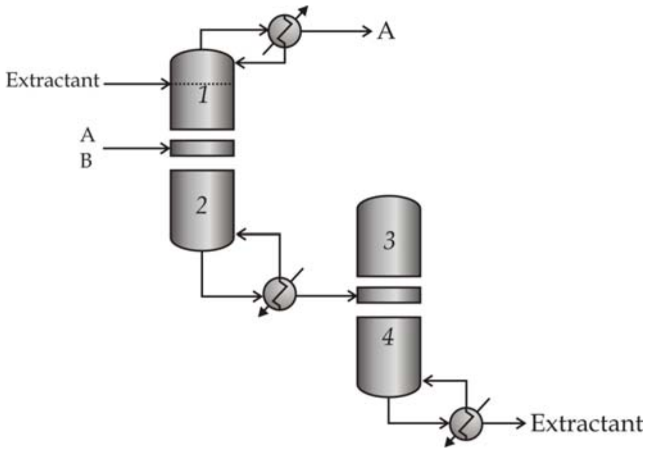

Figure 1: Conventional extractive distillation sequence (DS)

Gutierrez-Guerra et al. (2009) have proposed a design and optimization procedures for a thermally coupled extractive distillation scheme (TCEDS-SR; Figure 2). The results showed that the energy savings predicted in the complex extractive distillation sequence can be achieved with reductions in greenhouse gas emissions, higher thermodynamic efficiencies and diminution in the minimum total annual operating cost. In this work, we analyze the dynamic behavior of the cases of study designed in the mentioned paper and compare them to extractive conventional distillation arrangements.

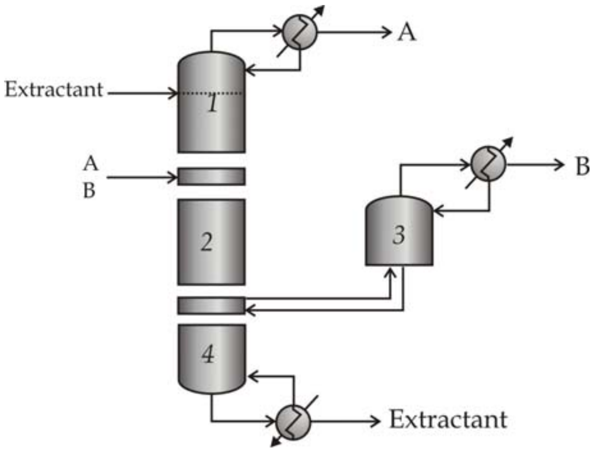

Figure 2:Thermally coupled extractive distillation sequence (TCEDS-SR)

2. OPEN LOOP ANALYSIS

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 singular value decomposition (SVD):

$$G = V\Sigma W^H \qquad (1)$$

where $\Sigma = \text{diag}(\sigma 1,\ldots\ldots,\sigma n)$, σi is the singular value of $G = (GG^H)$; $V = (v1, v2, \ldots\ldots)$ is the matrix of left singular vectors, and $W = (w1, w2, \ldots.)$ is the matrix of right singular vectors, respectively. Two parameters of interest are the minimum singular value, $\sigma*$, and the ratio maximum to minimum singular values, or better known as condition number:

$$\gamma = \sigma* / \sigma* \qquad (2)$$

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. In this case, we cover a sufficiently complete range of frequencies to analyze our case of study.

3. CLOSED LOOP ANALYSIS

One of the key parts for the dynamic analysis is the selection of control outputs and manipulated variables for each control loop. Although more formal techniques to define the control loops for the complex columns may be used (e.g., the relative gain array method for selecting the control loops in order to minimize the amount of interaction among the resulting loops), we based our selection on practical considerations. In the case of distillation columns, however, such loops are fairly well established and used successfully in practice, at least for conventional columns. A well-known structure is based on energy balance considerations, which yields to so-called LV control structure in which the reflux flowrate L and the vapor boilup rate V (which are affected directly by the heat duty supplied to the reboiler) are used to control the distillate and bottom outputs compositions. Thus, for any sequence, the control of the lightest component of the ternary mixture was manipulated with the top reflux flowrate. The control of the intermediate component was paired to the reflux flowrate of second column. In this study we do not analyze the control of entrainer (heavy component) due to in the industrial practice the control focuses principally on the components of the original binary mixture. The closed loop analysis was based on proportional-integral 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 (τi), 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.

4. CASE OF STUDY

We analyze the configurations designed in the work of Gutierrez-Guerra et al. (2009) where three ternary mixtures were considered (see Table 1). The UNIQUAC model was used to predict thermodynamic properties. Different extractant/feed (E/F) ratios were investigated. The design pressure for each separation was chosen to ensure the use of cooling water in the condensers. Purities of 99 % in mole in the products were assumed. As far as energy consumption is concerned, the optimized steady – state complex design provides energy savings of ~30% (and reduction in CO_2 emissions) with respect to the best energy – efficient sequence based on conventional extractive distillation columns.

Table 1: Mixtures Studied

Mixture	Feed Components	Feed Component Flows (kmol/h)	Mixture
M1	Tetrahydrofuran/Water	40.82/4.53	1,2-Propanediol
M2	Acetone/Methanol	45.35/45.35	Dimethyl sulfoxide (DMSO)
M3	n-Heptane/Toluene	90.72/90.72	Aniline

5. RESULTS

The controllability analysis was conducted in two parts. The theoretical control properties of the three schemes were first predicted through the use of the singular value decomposition (SVD) technique, and then closed-loop dynamic simulations were conducted to analyze the control behavior of each system and to compare those results with the theoretical predictions provided by SVD.

5.1 Singular Value Decomposition

The theoretical control properties of conventional and thermally coupled extractive distillation sequences were obtained. 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. Open – loop dynamic simulations were carried out in Aspen Dynamic in order to obtain the transfer function matrix. For the distillation sequences presented in this work, three controlled variables were considered: product composition A, B and C. Similarly, three manipulated variables were defined: the reflux ratios (in both columns) and reboiler duty. For the case of study considered here, Table 2 and 3 show some representative transfer function matrices generated by using step changes in the manipulated variable and recording the dynamic behavior of the three product compositions (A–C). The transfer function matrix shown in Table 2 corresponds to TCEDS–SR (M1; E/F=2.0). It can be observed that dynamic responses can be adjusted to first or second order or parallel processes. On the other hand, Table 3 shows the transfer function matrix for the DS (M1; E/F=2.0). Similar transfer function matrices can be obtained for all cases of study.

Table2: Transfer Function Matrix for TCEDS-SR (M1; E/F=2.0)

$$\begin{bmatrix} \dfrac{0.2174}{4.190\,s+1} & \dfrac{-\,0.001}{(0.332\,s+1)(0.856\,s+1)} & \dfrac{-\,0.0010}{0.828\,s+1} \\ \dfrac{72.0382}{(1.026\,s+1)(10.026\,s+1)} & \dfrac{71.4646}{(1.142\,s+1)(1.142\,s+1)} & \dfrac{-\,3.865}{(0.518\,s+1)(0.518\,s+1)} \\ \dfrac{-\,0.0001}{0.828\,s+1} & \dfrac{-\,0.0001}{0.828\,s+1} & \dfrac{0.7020}{2.594\,s+1} \end{bmatrix}$$

Table 3: Transfer function matrix for DS (M1; E/F=2.0).

$$\begin{bmatrix} \dfrac{0.2577}{(0.701s+1)(1.681s+1)} & \dfrac{0.0013}{24.762s+1} & \left(\dfrac{0.023}{3.857s+1}-\dfrac{0.1618}{1.772s+1}\right) \\ \dfrac{2.8522}{(1.951s+1)(1.951s+1)} & \dfrac{0.0723}{(5.087s+1)(0.793s+1)} & \left(\dfrac{4.2582}{5.119s+1}-\dfrac{4.2972}{17.179s+1}\right) \\ 0 & 0 & \dfrac{0.1324}{16.264s+1} \end{bmatrix}$$

For the case of study of TCEDS–SR and DS, we obtained the following results: for the case M1; E/F=2.0 (see results reported in Figures 3 and 4), the TCEDS-SR arrangement presents higher values of the minimum singular value and lower condition number for the entire frequency range; therefore, it can be expected that the TCEDS-SR system will exhibit better control properties than the other sequence under feedback control, and is better conditioned to the effect of disturbances than the other distillation scheme. Figures 5 and 6 show the minimum singular value and condition number for the case of study M1; E/F=2.5. The TCEDS–SR presents higher values of $\sigma*$ and lower values of γ for the entire frequency range. Therefore, the TCEDS–SR is expected to require less effort control under feedback operation and is better conditioned to the effect of disturbances than the conventional extractive scheme. For the case of M1; E/F=3.0, our results show that at low frequencies TCEDS–SR exhibits higher values of $\sigma*$ than the other scheme, but as the frequency increases, the minimum singular value is similar to the values of DS scheme. In the case of the number condition, TCEDS–SR shows the lowest values at low frequencies. In general, we can say that TCEDS–SR offers better conditioning properties for model uncertainties and process disturbances than the other arrangement at low frequencies. According to SVD for the case of M1; E/F=3.5, TCEDS–SR shows better control properties than conventional extractive arrangement, because that scheme presents lower values for condition number and similar minimum singular values in comparison with the DS arrangement. For the case M1, E/F=4.0, the SVD results are similar to the case E/F=3.5. Based on the trends observed, two distinctions are seen between the TCEDS-SR and DS: in general, the arrangement with thermal coupling is expected to require less control efforts under feedback operation and, as the E/F ratios are increasing, the control properties of the complex extractive scheme are similar to those of the conventional extractive scheme. On other words, at low values of E/F the coupled extractive columns present the best values of the minimum singular value and condition number in comparison to the values of the conventional extractive columns for what the best option to operate the complex arrangements is in those values of E/F ratios (~2.0 to 3.0).

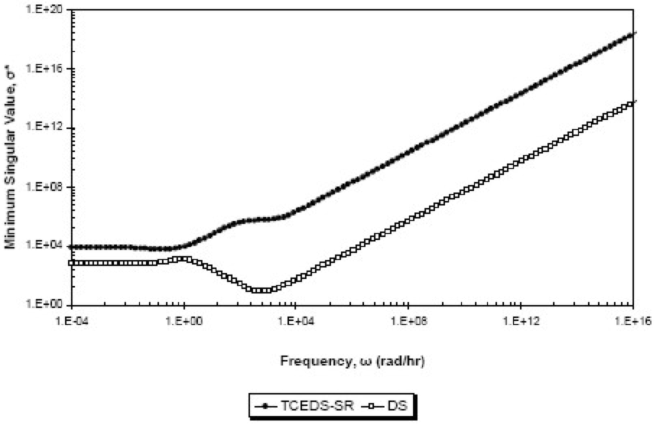

Figure 3: Minimum singular value, mixture M1 (E/F=2.0).

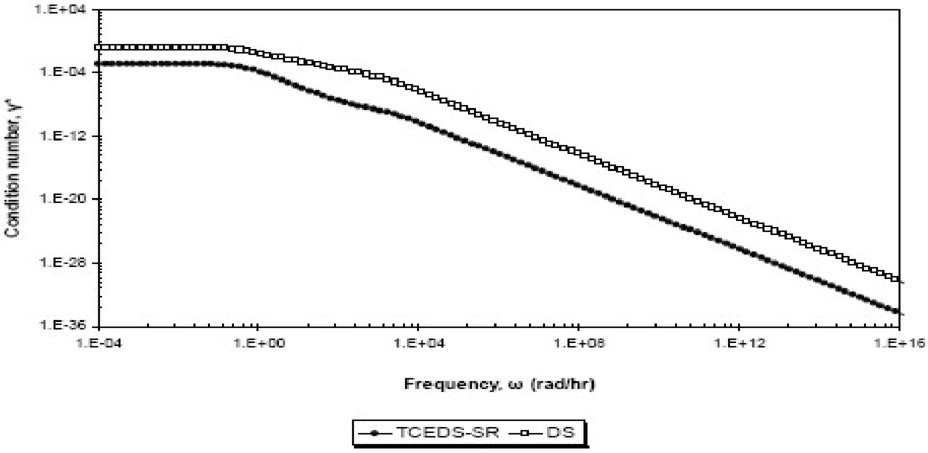

Figure 4: Condition number, mixture M1 (E/F=2.0)

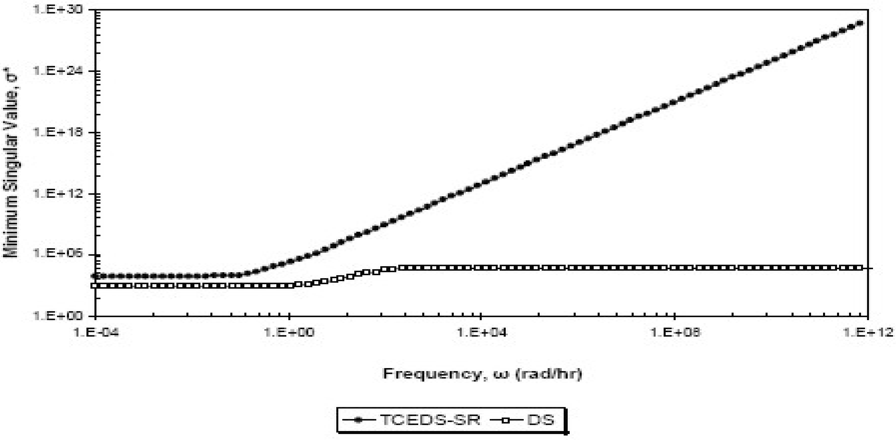

Figure 5: Minimum singular value, mixture M1 (E/F=2.5)

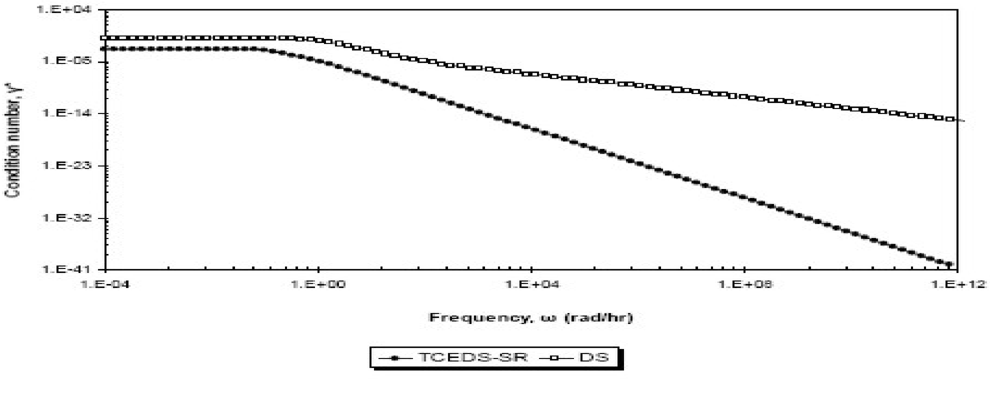

Figure 6: Condition number, mixture M1 (E/F=2.5).

Similar results can be obtained for case of study M2 and M3 and for all E/F options. In general, it can be concluded that TCEDS-SR presents better control properties than DS and the best option is the operation of the complex arrangements at low values of E/F ratios, in all cases of study. Also, the results indicate that the presence of interconnections, in coupled extractive systems, provide an improvement in controllability properties.

5.2 Closed-Loop Simulations

For the dynamic analysis, individual set point changes for product compositions were implemented for each of the two product streams (we do not analyze the closed loop for entrainer stream). For all cases (i.e., conventional and integrated extractive sequences), the two 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. Also, this part of the study was conducted with the use of Aspen Dynamics. Table 4 shows the IAE values obtained for each E/F ratio and for each control loop of the two distillation sequences for mixture M1. When the ratio E/F=2.0 was considered, TCEDS-SR system offered the best dynamic behavior, based on the lowest values of IAE, for the control of the two product streams, in comparison with the conventional extractive configuration. The control of the light or intermediate components does not create any significant problems in the case of complex system. However, one may notice how the conventional extractive sequence shows some oscillations before to get the settling time. These results are consistent with the values of IAE. In general, the thermally coupled extractive system offers the highest energy savings and also shows the best dynamic performance in comparison with DS arrangement under consideration. Table 4 shows the IAE values when the E/F ratio takes the value of 2.5. In this case, similar results to the case E/F=2.0 were obtained. The TCEDS-SR presents the lowest values of IAE. Due to these results, the complex system of separation is a better option that the conventional system of distillation. Both cases are in consistency with those obtained by means of SVD technique. When the E/F ratio was raised from 2.5 to 3.0 significant changes in the dynamic responses of the distillation systems were observed (see Table 4): IAE value for the control of the light component is the highest in the coupled system, while IAE value for the control of the component intermediate is the lowest in the coupled system. Similar results are obtained for the cases where E/F ratio takes values of 3.5 and 4.0. These last three analyzed cases show that the complex sequence is not the best option when the dynamic behavior is compared with the conventional arrangement. The conclusions obtained by means of SVD analysis (for the case M1) indicate that the best option to operate the complex systems was for low E/F ratios (~2.0 to 3.0). The results operating the sequences under closed loop fashion are in consistency with those estimated using the SVD technique. Similar results can be observed for the case of study N2 and M3. In general those results are also in consistency with the obtained ones by means of methodology of SVD: the best option to operate the thermally coupled extractive systems is for low E/F ratios.

6. CONCLUSIONS

We have conducted a comparison on the dynamic behavior of two extractive distillation sequences: case conventional and case thermally coupling. The dynamic analysis was based on SVD technique and PI controllers, for which the parameters were tuned up through a minimization procedure of the integral of the absolute error.

Table 4: IAE Results for Mixture M1

	Tetrahydrofuran			**Water**		
E/F=2.0						
Sequence	K_c	τ_i (min)	IAE	K_c	τ_i (min)	IAE
DS	14	1	5.725 E-4	500	15	1.658 E-4
TCEDS-SR	249	50	3.366 E-4	500	16	3.196 E-5
E/F=2.5						
Sequence	K_c	τ_i (min)	IAE	K_c	τ_i (min)	IAE
DS	42	2	6.116 E-4	500	525	9.140 E-5
TCEDS-SR	107	371	3.253 E-4	500	31	4.094 E-5
E/F=3.0						
Sequence	K_c	τ_i (min)	IAE	K_c	τ_i (min)	IAE
DS	57	1	6.714 E-4	500	370	1.110 E-4
TCEDS-SR	21	340	1.145 E-3	500	14	3.354 E-5
E/F=3.5						
Sequence	K_c	τ_i (min)	IAE	K_c	τ_i (min)	IAE
DS	500	122	1.144 E-4	500	399	2.389 E-4
TCEDS-SR	100	338	2.791 E-4	500	15	3.204 E-5
E/F=4.0						
Sequence	K_c	τ_i (min)	IAE	K_c	τ_i (min)	IAE
DS	500	99	2.329 E-4	500	434	1.269 E-4
TCEDS-SR	21	335	1.080 E-3	500	28	3.126 E-5

Our results indicate, in general, that the TCEDS-SR system is better than the DS scheme. It is apparent that the presence of recycle streams, instead of deteriorating the dynamic behavior of separation sequences, may contribute positively to their dynamic properties. Additional, the results suggest at low values of E/F the coupled extractive columns present the best values of the minimum singular value and condition number in comparison to the values of the conventional extractive columns for what the best option to operate the complex arrangements is in those values of E/F ratios. In summary, the present study shows that there are cases in which integrated extractive sequences do not only provide significant energy savings and reduction in CO_2 emissions with respect to the conventional extractive arrangements, but also may offer dynamic advantages.

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Brief Biography of the Presenter

Adrián Bonilla-Petriciolet is Professor in the Department of Chemical Engineering of Instituto Tecnológico de Aguascalientes, México. His research interests are applied thermodynamics, process design and optimization. He has published several papers in international journals and presented a number of papers in conferences.