16th European Symposium on Computer Aided Process Engineering
and 9th International Symposium on Process Systems Engineering
W. Marquardt, C. Pantelides (Editors)

# Controllability Analysis of Thermally Coupled Distillation Sequences for Five – Component Mixtures

Marcelino Carrera – Rodriguez, Minerva Ledezma – Martinez, Juan Gabriel Segovia-Hernández, Salvador Hernández

*Universidad de Guanajuato, Facultad de Química, Noria Alta s/n, Guanajuato, Gto., 36050, México, gsegovia@quijote.ugto.mx*

## Abstract

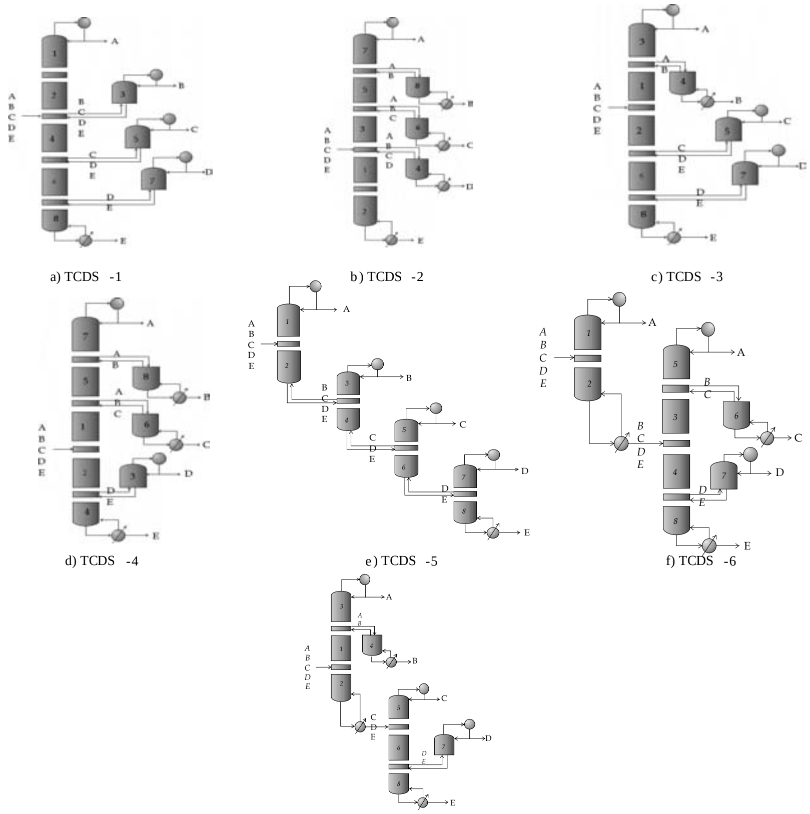
The control properties of thermally coupled distillation sequences for the separation of five – component mixtures of hydrocarbons were compared to those of conventional distillation sequences. Seven thermally coupled arrangements were investigated. The preliminary steady – state designs of complex schemes were obtained by starting from conventional distillation sequences and then optimizing for minimum energy consumption. The control properties of the sequences considered were obtained by using the singular value decomposition technique at zero frequency and analyzing rigorous dynamic simulations. It was found that, in general, the coupled schemes present theoretical control properties similar or better than those of conventional distillation sequences. This result establishes that the energy savings predicted for thermally coupled distillation sequences can be achieved in practice.

## 1. Introduction

Effective screening of separation systems constitutes a critical stage, as engineers need to review and understand trade-offs ahead of detailed modeling and simulation. In the separation, it is often desired to explore the use of complex rather than simple columns, because the complex units reduce mixing losses, use available vapor and liquid more effectively, and improve the separation efficiency (Hernández *et al*, 2003). Among all possible complex schemes for multicomponent distillation process, the thermally coupled distillation sequences are very promising for both energy and capital cost savings. However, due to the complexity, research on these complex distillation configurations is only restricted to three – component mixtures, for only a few promising flowsheets that can be constructed for ternary mixtures (Tedder and Rudd, 1978; Hernández and Jiménez, 1996). In these studies, it has been reported that the thermally coupled configurations are capable of achieve energy savings of up to 30% in contrast to the conventional direct and indirect distillation sequences. There are few works on extensions toward the design of integrated systems for mixtures of more than three components (Christiansen *et al.,* 1997; Blancarte-Palacios *et al*., 2003). Recently, Rong *et al* (2000; 2003) have parametrically studied some thermally coupled distillation sequences for five – component mixtures from viewpoint of economic evaluation and optimal synthesis of the multicomponent thermally coupled distillation flowsheets. The expectance that the dynamic properties of those coupled systems may cause more operational problems than the conventional sequences is one of the factors that have contributed to their lack of industrial implementation. In this work we developed a comparative study of the control properties between seven thermally coupled distillation sequences (previously studied by Calzon - McConville *et al.,* 2006) and seven conventional distillation sequences (Figures 1 – 7) for the separations of five – component mixtures.

## 2. Design and optimization strategies

Strictly, the design of the thermally coupled distillation sequences could be modeled through superstructures suitable for optimization procedures with mathematical programming techniques. However, the task is complicated and is likely to fail to achieve convergence. In this work, in order to overcome the complexity of the simultaneous solution of the tray arrangement and energy consumption within a formal optimization algorithm, we have decoupled the design problem in two stages: (1) tray configuration; (2) energy-efficient design (optimal energy consumption). In the first stage, our approach begins with the development of preliminary designs for the complex systems based on the designs of the conventional distillation sequences (as proposed by Hernández and Jiménez, 1996). For the conventional sequences, it is assumed that each column performs its respective split (i.e., the separation of the light and heavy key components) with molar recoveries of 98% respectively. Then, by using the shortcut method of Fenske-Underwood-Gilliland, the tray structures of conventional distillation schemes are obtained. After the tray arrangements for the integrated designs have been obtained, an optimization procedure is used to minimize the heat duty supplied to the reboilers of each coupled scheme; taking into account the constraints imposed by the required purities of the five products streams. The resulting sections serve as a basis for the tray arrangements of the complex scheme.



a) TCDS -1 b) TCDS -2 c) TCDS -3

d) TCDS -4 e) TCDS -5 f) TCDS -6

g) TCDS -7

Figure 1. Thermally coupled distillation sequences (TCDS) for separation of five component mixtures.

The remaining degrees of freedom (the number of thermal links; see Figure 1) after design specifications and tray arrangement are used to obtain the proper values of the interconnecting vapor streams which provide minimum energy consumption. In this work, the process simulator Aspen Plus 11.1$^{TM}$ is used for this purpose. If the product compositions are obtained, then the design is kept; otherwise, proper adjustments must be made. The values of the interconnecting flows are optimized for minimum energy consumption in the reboilers (more details about the procedure are in Calzon – McConville *et al*., 2006).

## 3. Theoretical Control Properties

Open loop dynamic responses 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 11.1$^{TM}$. Transfer function matrices (G) were then collected for each case, and they were subjected to singular value decomposition (SVD):

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

where $\Sigma$ = diag ($\sigma_1$,.....,$\sigma_n$), $\sigma_i$ = singular value of G = $\lambda_i^{1/2}(GG^H)$; V = ($v_1$, $v_2$,…..) matrix of left singular vectors, and W = ($w_1$, $w_2$,….) matrix of right singular vectors. Two parameters of interest are the minimum singular value, $\sigma_*$, and the ratio maximum to minimum singular values, or condition number ($\gamma^*$). The minimum singular value is a measure of the invertibility of the system and represents a measure of potential problems of the system under feedback control. The condition number reflects the sensitivity of the system under uncertainties in process parameters and modelling errors. These parameters provide a qualitative assessment of the theoretical control properties of the designs. The systems with higher minimum singular values and lower condition numbers are expected to show the best dynamic performance under feedback control. For this initial analysis, we simply estimated the SVD properties for each separation system at zero frequency. Such analysis should give some preliminary indication on the control properties.

## 4. Case of Study

The components of the mixtures considered are n-butane, n-pentane, n-hexane, n-heptane and n-hexane for mixture 1, and n-butane, isopentane, n-pentane, n-hexane and n-heptane for mixture 2. Two molar compositions F1 (A=0.35, B=0.1, C=0.1, D=0.1, E=0.35) and F2 (A=0.125, B=0.25, C=0.25, D=0.25, E=0.125) for each mixture are analyzed. Molar recoveries of 98, 94, 94, 94 and 97 are assumed for each component in the products. A feed flowrate of 45.5 kmol/h as saturated liquid is used. The operational pressure for each column is chosen in order to guarantee the use of cooling water in the condensers. As far as energy consumption is concerned, the optimized steady – state design provides energy savings of ~35% with respect to the best energy – efficient sequence based on conventional distillation columns.

## 4. Results

Table 1 presents the results for the SVD test for each sequence. The TCDS – 1 option has similar values of minimum singular value and condition number to those of the conventional sequence (CS – 1), which implies that the coupled arrangement has similar control properties (lower control efforts under feedback operation and better conditioned to the effect of disturbances) that the conventional design. The TCDS – 2, TCDS – 3, TCDS – 4, TCDS – 6 and TCDS – 7 systems present higher values of the minimum singular value; therefore, it can be expected that these coupled systems exhibit better control properties than the conventional sequences under feedback control. The results for the condition number show that the complex sequences offer the best values. As a result, it can be expected that thermally coupled distillation systems are better conditioned to the effect of disturbances than the conventional arrangements.

Table 1 Dynamic properties of the distillation systems.

| Sequence | $\sigma_*$ | $\gamma$ | IAE (Component A) |
|---|---|---|---|
| CS - 1 | 0.0219 | 562.85 | $1.4879 \times 10^{-5}$ |
| TCDS - 1 | 0.0218 | 564.29 | $1.4751 \times 10^{-5}$ |
| CS - 2 | 0.0012 | 14106 | $4.0077 \times 10^{-4}$ |
| TCDS - 2 | 0.2026 | 33.37 | $5.4113 \times 10^{-5}$ |
| CS - 3 | 0.0005 | 33318 | $6.8872 \times 10^{-4}$ |
| TCDS - 3 | 0.0418 | 576.8 | $3.0709 \times 10^{-5}$ |
| CS - 4 | 0.0064 | 59934 | $2.0089 \times 10^{-4}$ |
| TCDS – 4 | 0.0071 | 56650 | $1.9999 \times 10^{-4}$ |
| CS - 5 | 0.0350 | 562.85 | $9.9784 \times 10^{-5}$ |
| TCDS – 5 | 0.0001 | 14000 | $5.3308 \times 10^{-4}$ |
| CS - 6 | 0.00220 | 13588 | $7.6608 \times 10^{-4}$ |
| TCDS - 6 | 0.00500 | 2630.14 | $6.9002 \times 10^{-4}$ |
| CS - 7 | 0.00003 | 19004 | $8.5508 \times 10^{-4}$ |
| TCDS - 7 | 0.00009 | 1973.8 | $8.0078 \times 10^{-4}$ |

Two details are worth highlighting, the TCDS – 1 and TCDS – 5 are thermodynamic equivalents schemes. The results (Table 1) show that TCDS – 5 have the worst control properties in comparison with the TCDS 1. This result is important because two thermodynamically equivalent schemes have different dynamic properties: the structure with side columns have better control properties than a thermodynamic scheme with retrofit. Some authors have claimed that the reduction of interconnection flows in complex arrangements might provide better operating properties. When we do a general comparison of control properties of the seven coupled scheme, the partially thermally coupled (TCDS 6 – 7) arrangements show worst values (minimum singular value and condition number) than the fully thermally coupled schemes (TCDS 1 – 4). This observation is interesting because the number of the thermal links affect the control properties of coupled systems. Similar results were obtained using dynamic simulations (Table 1). The IAE criterion shows the best dynamic behavior for the thermally coupled distillation sequences using PI controllers (Table 1). For the dynamic analysis, individual set point changes for product composition were implemented for each of the three product streams. For all cases (conventional and integrated sequences), the five control loops were assumed to operate under closed loop fashion

## 5. Conclusions

It has been shown that the controllability properties of seven thermally coupled distillation sequences for the separation of five component mixtures are better than those of the conventional sequences. The results show that the structure has different effect to dynamic performance for a specific separation in the case of thermodynamically equivalent schemes. These results are significant because they let us establish that coupled schemes not only require energy demands lower than the conventional distillation sequences but also present control properties similar or better to those of the conventional distillation sequences used in the preliminary design of the thermally coupled distillation sequences. 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.

## 6. References

Blancarte – Palacios, J.L., Bautista – Valdés, M.N., Hernández, S., Rico – Ramírez, V., and A. Jiménez, 2003, *Ind. Eng. Chem. Res.*, 42, 5157.

Calzon – McConville, C.J., Rosales – Zamora, M.B., Segovia – Hernández, J.G., Hernández, S., and V. Rico – Ramírez, 2006, *Ind. Eng. Chem. Res.*, 45, 724.

Hernández, S., and A. Jiménez, 1996, *Trans IChemE*, 74, 357.

Hernández, S, Pereira-Pech, S, Jiménez, A, and V. Rico-Ramírez, *The Can. J. Chem. Eng*. 2003; 81 (5) 1087.

Rong B. G., Kraslawski, A., and L. Nystrom, 2000, *Comput. Chem. Eng.*, 24, 247

Rong B. G., and A. Kraslawski, 2003, *Ind. Eng. Chem. Res.*, 42 (6), 1204.

Tedder, D.W., and D.F. Rudd, 1978, *AIChE J*, 24, 303.

## Acknowledgements

The authors acknowledge financial support received from PROMEP and Universidad de Guanajuato, México