17th European Symposium on Computer Aided Process Engineering – ESCAPE17
V. Plesu and P.S. Agachi (Editors)

Design and control analysis of thermally coupled configurations for quaternary distillations

Juan Gabriel Segovia – Hernández[a], Jesús Rafael Alcántara –Ávila[a], Julián Cabrera – Ruiz[a], Salvador Hernández[a], Ben - Guang Rong[b]

[a]*Universidad de Guanajuato, Facultad de Química, Noria Alta s/n, Guanajuato, Gto., 36050, México. gsegovia@quijote.ugto.mx*
[b] *Department of Chemical Technology, Lappeenranta University of Technology, P.O. Box 20, Fin – 53851, Lappeenranta, Finland.*

Abstract

In this work we developed a comparative study of the energy consumption, thermodynamic efficiency, total annual costs and control properties (using the singular value decomposition technique in the frequency domain) of five thermally coupled distillation sequences for the separations of quaternary mixtures. The results show that the structure has different effects on energy consumption, capital costs and dynamic performance. These results are significant because they let us establish that coupled schemes not only require lower energy demands and have better thermodynamic efficiencies than the conventional distillation sequences but also present theoretical control properties similar or better to those of the conventional distillation sequences used in the preliminary design of the thermally coupled distillation sequences.

Keywords: thermally coupled distillation sequences, energy savings, control properties.

1. Introduction

Distillation is the most widely used separation technique in the process industry; its main disadvantage is the high consumption of energy that often represents a high percent of the total energy cost of the plant. The energy saving in distillation is then an essential field of the chemical engineering research. As a result, one trend in process design is to utilize separation schemes different from the sequences of simple columns, in particular, that can provide significant reductions of heat requirements [1-2]. The thermal coupling between two columns in a sequence can be adopted to reduce the energy consumption of the process [3]: the use of complex distillation sequences, such as the thermally coupled ones, for the separation of multicomponent mixtures can offer energy savings around 30% with respect to the conventional distillation trains [4]. Thermally coupled schemes, especially for the separation of ternary mixtures, have been proposed for some time. Despite the potential benefits of thermally coupled columns and some reports of successful industrial applications only a limited number of such columns has been implemented in the field, mainly because of complexity in design and control of these structures [5] since the flexibility and the controllability of those systems depend strongly on the number of units and their interconnections. In industrial processes, the mixtures to be separated often contain four or more components. There are few works on extensions toward the design and control properties of integrated systems for mixtures of more than three components as reported by Rong *et al.*, [6] there are many thermally coupled distillation sequences for the separation of quaternary mixtures. Each scheme has different structure and different dynamic properties. The reason is that each thermal coupling would have different effect on steady state as well as dynamic performance for a specified separation. In this work, we analyze the conventional sequence of $AB/CD \rightarrow A/B \rightarrow C/D$ (CS; Fig. 1) and propose the following five different complex designs: (a) TCDS-I: just eliminate condenser in section 1 (Fig. 1) and introduce one thermal coupling (Fig. 2a); (b) TCDS-II: move column section 3 to the top of column, section 1, in CS (Fig. 2b); (c) TCDS-III: just eliminate reboiler in section 2 (Fig. 1) and introduce one thermal coupling CD (Fig. 2c); (d) TCDS – IV: move column section 6 to the bottom of column, section 2, in CS (Fig. 2d); (e) TCDS – V: eliminate both condenser and reboiler in section 1 and 2 of CS and introduce both thermal coupling (Fig. 2e). In these columns we developed a comparative study of the energy consumption, thermodynamic efficiency, total annual costs and control properties. The results show that the structure has different effect on energy consumption, capital costs and dynamic performance.

2. Design and dynamic study of complex arrangements

The first step for this analysis consists in the detection of a base design for the integrated arrangements. The design of such schemes was carried out through a section analogy procedure, taking as a basis the tray structure of the conventional sequence given in Figure 1. The conventional system contains six sections; those tray sections can also be identified within the structure of the complex sequences (Figure 2), thus providing the basis for the tray arrangement of the interconnected structure.

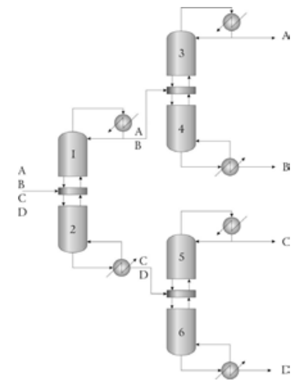
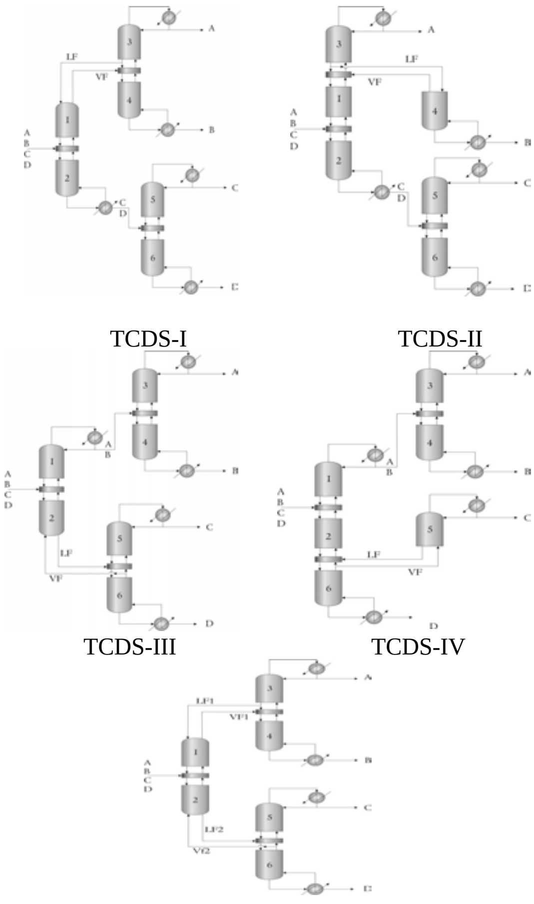


Figure 1. Conventional distillation Sequence with prefactionator (CS).



TCDS-V

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

After the base designs for the TCDS structures were obtained, a search procedure on the interconnection streams (VF, LF or both) was carried out until the minimum energy consumption was detected for each case. Further details on the design and optimization method are available in Blancarte-Palacios *et al.* [7]. We complement the study calculating the total annual cost (TAC) and second law efficiency (η) in those schemes. Such resulting structures with minimum energy consumption provided the designs that were subjected to the dynamic analysis. Open loop dynamic responses to set point changes around the assumed operating point were obtained. Transfer functions were grouped into a transfer function matrix (G) and they were subjected to singular value decomposition (SVD). Two parameters of interest are the minimum singular value, σ_*, and the ratio maximum (σ^*) to minimum singular values, or condition number (γ^*). 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. 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. To compare the performance of the integrated arrangements with the conventional sequence, three four-component mixtures of n-butane, n-pentane, n-hexane and n-heptane (M1); benzene, toluene, ethyl-benzene and o-xylene (M2); i-butane, n-butane, i-pentane and n-pentane (M3) were considered, with a feed flowrate of 45.5 kmol/hr, and two composition: (0.40/0.10/0.10/0.40; F1) and (0.10/0.40/0.40/0.10; F2) mole fraction. The specified product purity for components A, B, C and D were 98.7, 98, 98 and 98.6 %, respectively. One aspect to be defined for the feedback control analysis is the selection of the control loops for the product composition streams, we based our selection on potential practical considerations (See Figure 3).

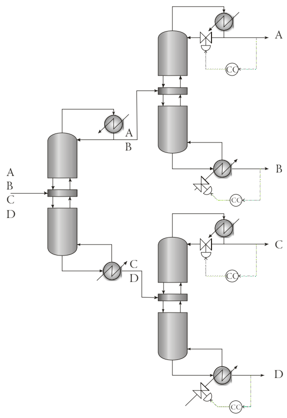


Figure 3. Control loops based in practical considerations in CS .

The manipulated variables for the TCDS were the corresponding reflux flowrates for the composition control of A and C, while the reboiler heat duties were used for the control of B and D. For the initial exploration of the dynamic behavior of the integrated sequences under analysis, PI controllers were selected for each loop. We used the minimization of the integral of the absolute error (IAE) as the criterion for controller tuning and the detection of best behavior.

3. Results

Table 1 shows the energy requirements for the separation of mixture M1, F1. The results indicate that the thermally coupled distillation sequences can offer energy savings between 10 and 40 % in contrast to the best conventional distillation option (CS). The efficiency in the use of the energy is better in the thermally coupled distillation sequences for the case of the separation of mixture M1. As indicated in Table 1, the second law

efficiency is increased through the use of thermal links. In all mixtures and compositions the results show similar trends.
It was obtained that the thermal links increase both energy savings and the second law efficiency.

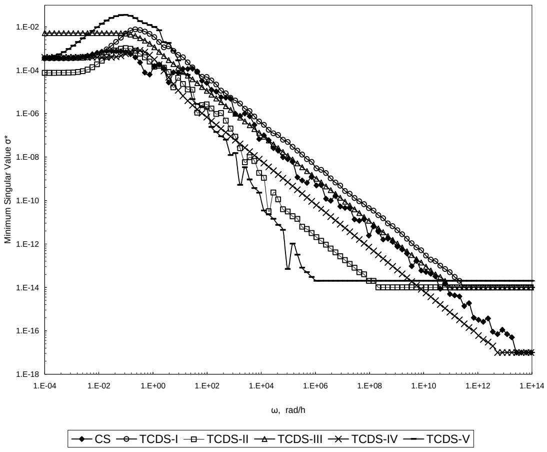


Figure 4. Minimum singular value for all schemes with mixture M1, F1.

Table 1. Energy consumption, total annual cost and thermodynamic efficiency (case M1F1).

Arrangement	Optimum Interconnection flowrate, (Lbmol/hr)	Energy consumption, (BTU/hr)	TAC, ($/yr)	η, (%)
CS	---	5,793,805.67	1,132,804	12.02
TCDS-I	LF= 68.00	5,304,488.81	979,610	13.15
TCDS-II	LF= 37.00	2,412,427.45	781,508	21.13
TCDS-III	VF= 165.00	4,798,480.47	956,179	15.08
TCDS-IV	VF= 137.00	3,645,163.12	990,869	19.67
TCDS-V	LF= 62.60 VF= 121.70	4,733,673.25	963,960	14.24

The results can be summarized as follows: the results indicate that the thermally coupled distillation sequences can offer energy savings between 10 and 40 % in contrast to the conventional distillation option (CS). This situation is function of the mixture and composition in the feed. The efficiency (η) in the use of the energy, in comparison with CS, is better or similar in the thermally coupled distillation sequences TCDS - I and TCDS - II are thermodynamically equivalent structures. In all cases the results show similar energy consumption and η. TCDS – III and TCDS – IV are thermodynamically equivalent arrangements. The results displayed show similar energy consumption and η. In all cases the complex distillation sequences have the lowest values of TAC. In general TCDS I or its thermodynamically equivalent structure show the lowest values of energy consumption, in comparison with CS. For the case M1F1 we got the next results: TCDS - I and TCDS - III presents, in general, lower condition number and higher values of the minimum singular; therefore, it can be expected that TCDS - I and TCDS - III systems exhibit better control properties than the other sequences under feedback control and it is better conditioned to the effect of disturbances than the other distillation schemes (Figure 4). As the frequency increases TCDS – II presents good dynamic behavior. However, TCDS – II and TCDS – V, at low frequencies, show the worst results. Similar results were obtained in all cases of study.The change of the topology affect the dynamic properties (TCDS – II and IV) of the complex arrangements. To supplement the SVD analysis, rigorous dynamic simulations under closed loop operation were carried out. 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. These results are similar to SVD analysis, in all cases, when we use feedback control analysis with PI controllers.

4. Conclusions

We have conducted a comparison on the energy consumption, η, TAC and dynamic behavior of five complex distillation sequences for the separation of quaternary mixtures. One factor seems to affect the optimal choice: the structure of the complex sequence. Schemes with change in their structural topology in comparison with CS have best energy savings. However, if the schemes do not have change in their topology, they can show best dynamic behavior. On the other hand, in some cases the utilities required in the reboilers of complex systems are more expensive because of their higher operational pressures. In summary, although the best operational option is not unique, the results show that there are cases in which integrated sequences do not only provide significant energy savings with respect to the conventional sequences, but also may offer some dynamic advantages.

Acknowledgements

Financial support from Universidad de Guanajuato is gratefully acknowledged.

References

1. Triantafyllou, C., and Smith, R., 1992, *Trans Inst. Chem. Eng.*, 70, 118.
2. Hernández, S., and Jiménez, A., 1996, *Trans IChemE*, 74, Part A, 357.
3. Rong, B.G., and Kraslawski, A., 2002, *Ind. Eng. Chem. Res.*, 41, 5716.
4. Tedder, D.W., and Rudd, D.F., 1978, *AIChEJ*, 24, 303.
5. Kaibel, B., Jansen, H., Zich, E., Olujic, Z., 2006, *In Distillation and Absorption '06, IChemeE Symp. Series No. 15*, 610.
6. Rong, B.G., Kraslawski, A., and Turunen, I., 2003, *Ind. Eng. Chem. Res.*, 42, 1204.
7. Blancarte – Palacios, J.L., Bautista – Valdés, M.N., Hernández, S., Rico – Ramírez, V., and Jiménez, A., 2003, *Ind. Eng. Chem. Res.*, 42, 5157.