19th European Symposium on Computer Aided Process Engineering – ESCAPE19
J. Jeżowski and J. Thullie (Editors)

Design and Optimization of Thermally Coupled Extractive Distillation Sequences

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Abstract

In this paper, design and optimization procedures are developed for a conventional extractive distillation sequence and a thermally coupled extractive distillation scheme. The proposed methodologies detect the optimal values of the design variables in order to guarantee the minimum energy consumption. It was found that the optimum energy consumption can be related to the minimum total annual operating cost, minimum greenhouse gas emissions, higher thermodynamic efficiencies and good theoretical control properties. The methodologies were applied to the study of the separation of several close boiling point mixtures using the two distillation sequences. The results showed that the energy savings predicted in the complex extractive distillation sequence can be achieved along with reductions in greenhouse gas emissions.

Keywords: CO_2 emissions, extractive thermally coupled distillation, energy savings.

1. Introduction

Distillation, which is the workhorse of chemical process industries, is an energy-intensive process, and is therefore among the first processes to be addressed to achieve energy savings over the short and long term. Energy consumption in distillation and greenhouse gas emissions (e.g. carbon dioxide) are strongly related. Reducing CO2 emissions is an absolute necessity and an expensive challenge in the chemical process industries, required to meet environmental targets as agreed in the Kyoto Protocol. Therefore, the reduction of CO2 emissions from distillation systems is an important issue, and much effort should be focused on energy savings techniques [1]. Most modifications and research efforts have been aimed principally at increasing heat integration within the distillation unit; some have been made directly to the heating device systems, while others have been performed on the main distillation columns. In particular, the use of columns with thermal coupling has received considerable attention in recent years, with a special development reported for the case of separation problems of ternary mixtures. Thermally coupled distillation systems (TCDS) are obtained through the implementation of interconnecting streams (one in the vapor phase and the other one in the liquid phase) between two columns; each interconnection replaces one condenser or one reboiler from one of the columns, thus providing potential savings in capital investment. Furthermore, through proper selection of the flow values for the interconnecting streams of TCDS, one can obtain significant energy savings (and, consequently, reductions in CO2 emissions) with respect to the energy consumption of conventional distillation sequences. There is a considerable amount of literature analyzing the relative advantages of TCDS for ternary separations [2]. These studies have shown that those thermally coupled distillation schemes are capable of typically achieving 30% energy savings over conventional schemes.

Azeotropic and low-relative volatility mixtures are commonly encountered in the fine-chemical and specialty industries, and many chemical processes depend on efficient and economical methods for their separation. These mixtures can be separated in a distillation column by altering the relative volatilities or shifting the azeotropic point to a more favorable position. Extractive distillation is defined as distillation in the presence of a miscible, high boiling, relatively non-volatile component, the solvent, which forms no azeotrope with the other components in the mixture. The method is used for mixtures having a low value of relative volatility, nearing unity. Such mixtures can not be separated by simple distillation, because the volatility of the two components in the mixture is nearly the same, causing them to evaporate at nearly the same temperature at a similar rate, making normal distillation impractical. The method of extractive distillation uses a separation solvent, which is generally nonvolatile, has a high boiling point and is miscible with the mixture, but does not form an azeotropic mixture. The solvent interacts differently with the components of the mixture thereby causing their relative volatilities to change. This enables the new three-part mixture to be separated by normal distillation. The original component with the greatest volatility separates out as the top product. The bottom product consists of a mixture of the solvent and the other component, which can again be separated easily because the solvent does not form an azeotrope with it. The bottom product can be separated by any of the methods available. It is important to select a suitable separation solvent for this type of distillation. The solvent must alter the relative volatility by a wide enough margin for a successful result. The quantity, cost and availability of the solvent should be considered. The solvent should be easily separable from the bottom product, and should not react chemically with the components or the mixture, or cause corrosion in the equipment. Extractive distillation is widely used in several different processes: i) recovery of aromas or fragances; ii) separation of aqueous alcohol solutions; iii) mixtures which exhibit an azeotrope and iv) separation of hydrocarbons with close boiling points [3]. In this paper we study the purification of several mixtures (only feasible the separations with extractive distillation) using the thermally coupled extractive distillation scheme with side rectifier (TCEDS-SR; Figure 1). Design, optimization and control properties were obtained for the examined complex configurations. The results show that the thermally coupled configuration is a better option than the conventional extractive distillation sequence (Figure 2) in terms of energy savings (reductions in greenhouse gas emissions) and capital investment.

2. Design of Complex Distillation Schemes

To overcome the complexity of the simultaneous solution of the tray arrangement and energy consumption within a formal optimization algorithm, we decoupled the design problem in two stages: (i) tray configuration; (ii) optimal energy consumption. The first stage of our approach begins with the development of preliminary designs for the complex systems starting from the design aspects of conventional distillation columns.

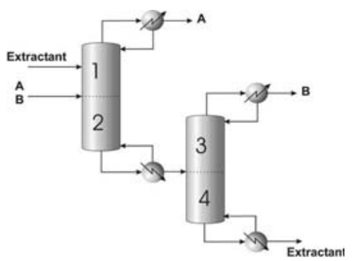


Figure 1. Conventional extractive distillation sequence (DS).

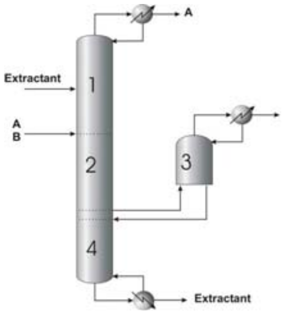


Figure 2. Thermally coupled extractive Distillation sequence (TCEDS-SR).

The design of the TCEDS-SR column is obtained by using a thermal link in the vapor phase in the conventional direct sequence (DS), which eliminates the reboiler in the second column of the conventional scheme, and the tray section (named section 4) is moved to the bottom of the first column of the conventional scheme (Figures 1 and 2). After the tray arrangement for the TCEDS-SR sequence has been obtained, an optimization procedure is used to minimize the heat duty supplied to the reboiler of the complex scheme, taking into account the constraints imposed by the required purity of the three product streams. Next, the degrees of freedom that remain after design specifications and tray arrangement are used to obtain the operating conditions that provide minimum energy consumption. Two degrees of freedom remain for the complex sequence. They are the side stream flow and the extractant stream stage.

The optimization strategy can be summarized as follows: (a) A base design for the complex scheme is obtained. (b) Values for the extractant stream stage and interconnecting flow are assumed. (c) A rigorous model for the simulation of the complex scheme with the proposed tray arrangement is solved. In this study, Aspen Plus One^{TM} was used for this purpose. If product compositions are obtained, then the design is kept; otherwise, appropriate adjustments must be made. (d) One value of side stream flow is changed, going back to step (c) until a local minimum in energy consumption for the assumed value of the side stream stage is detected. (e) The value of extractant stream stage is modified, going back to step (c) until the energy consumption is minimum (optimization criterion). This result implies that an optimum value has been detected for the design of the complex scheme.

3. Case of Study

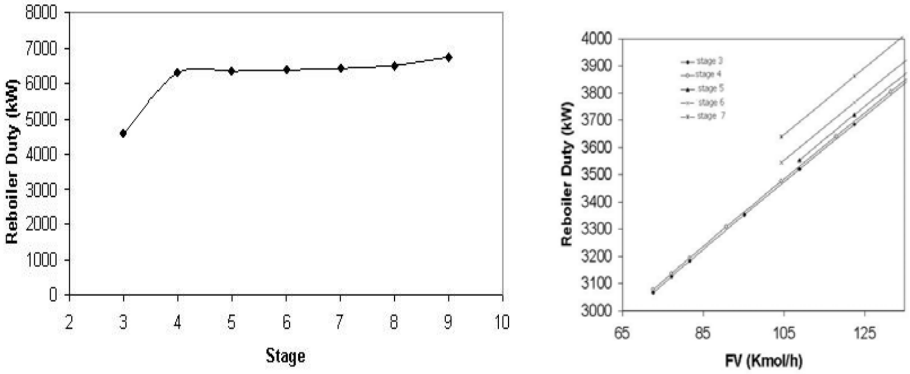
To compare the behavior of the sequences, three ternary mixtures were considered (Table 1). The number of ideal stages, the feed stage and the initial extractant stage in the thermally coupled extractive distillation sequence were set after the optimization of the structure of the conventional direct sequence was carried out. These parameters enabled a successful separation. 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.

Table 1. Mixtures analyzed.

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

4. Results

The resulting designs and their performance with respect to energy consumption, CO_2 emissions [1], thermodynamic efficiency [4] and total annual cost (TAC) are discussed. Typical optimization curves for the DS and TCEDS-SR (case M2) are shown in Figures 3a and 3b, respectively, where the optimal value for the extractant stage can be determined for the DS, and for the case of the TCEDS-SR both values of the extractant stage and interconnecting flowrate can be detected in order to guarantee minimum energy consumptions. The optimization curves show an interesting effect of the search variables on energy consumption. The design is sensitive, in terms of its energy consumption, to changes in interconnecting flowrates and extractant stage. An implication of this observation has to do with operational considerations (the presence of recycle can contribute in a well dynamic behavior).



a) DS b) TCEDS-SR

Figure 2. Search for the minimum energy consumption of the designs.

Tray arrangements and some important design variables for that sequence after the optimization task are given in Tables 2. The results of the rigorous optimization are collected in Table 3 for the extractive distillation configurations, indicating the effect of solvent feed ratio (E/F) on energy consumption, economic evaluation, second law efficiency and CO_2

Table 2. Design variables for TCEDS-SR (M1; E/F=2.0).

	Main Column	Side Rectifier
Pressure (atm)	1.14	1.14
Stages	33	17
Feed Stage	17	
Extractant Stage	3	
Interconnection Stage	24	
FV (kmol/h)	4.98	

Table 3. Results for different extractant/feed ratios, case M1.

		E/F = 2.0		
Sequence	Energy Consumption (kW)	TAC ($/yr)	η	CO_2 Emissions (Ton/h)
DS	2264.11	827,624.71	48.40	0.62
TCEDS-SR	1719.49	656,333.29	32.08	0.47
		E/F = 2.5		
Sequence	Energy Consumption (kW)	TAC ($/yr)	η	CO_2 Emissions (Ton/h)
DS	2463.47	887,466.55	27.95	0.68
TCEDS-SR	1823.18	686,478.34	37.58	0.50
		E/F = 3.0		
Sequence	Energy Consumption (kW)	TAC ($/yr)	η	CO_2 Emissions (Ton/h)
DS	2711.0	962,586.56	30.20	0.74
TCEDS-SR	1943.06	721,606.88	42.15	0.53
		E/F = 3.5		
Sequence	Energy Consumption (kW)	TAC ($/yr)	η	CO_2 Emissions (Ton/h)
DS	2968.30	1,040,571.40	31.95	0.81
TCEDS-SR	2088.39	764,676.89	45.62	0.57
		E/F = 4.0		
Sequence	Energy Consumption (kW)	TAC ($/yr)	η	CO_2 emissions (Ton/h)
DS	3228.83	1,119,517.07	33.39	0.89
TCEDS-SR	2243.70	810,951.68	48.41	0.62

For all cases of study, the results can be summarized as follows: (i) reducing solvent feed ratio of the complex extractive distillation systems causes a reduction of energy savings in comparison with the conventional distillation sequence, and consequently the total annual cost will be increased; (ii) the energy savings achieved by complex extractive schemes are in the range between 20 and 30% in contrast to the conventional arrangement; (iii) the second law efficiency (η) of the TCEDS-SR is higher than that of the corresponding conventional extractive distillation option; (iv) the reduction in global CO_2 emissions, in TCDES-SR, is considerable: in the range between 24 and 30%. The inefficiency of conventional sequences (associated with CO_2 emissions) has been reported as a consequence of remixing [2]. Therefore, proper optimization of the thermally coupled extractive sequence should avoid such a remixing problem. The methodology proposed generates designs where the effect of the remixing is eliminated. In general, the results show that the optimization of the thermal link causes significant energy savings, TAC savings and reduction in CO_2 emissions, and improves the values of second law efficiencies (especially at high values of E/F). Those results also were observed in other cases of study.

5. Conclusions

The design and optimization of a thermally coupled extractive distillation sequence with side rectifier were studied and compared to those of a conventional extractive distillation sequence. A general energy-efficient design procedure has been used that accounts for CO_2 emissions from the TCEDS-SR. The approach optimizes all process conditions in order to achieve energy savings and reductions in CO_2 emissions. Examples have shown that the design procedure can provide all of the operating parameters needed. Some trends were observed: TCEDS-SR presented energy savings (and TAC savings) between 20 and 30% over conventional schemes. The complex scheme presents a reduction in carbon dioxide emissions. The results imply that the proposed extractive thermally coupled distillation sequence can achieve significant energy savings that can be translated into reductions of CO_2 emissions.

6. Acknowledgements

We acknowledge the financial support provided by Universidad de Guanajuato, CONACyT and CONCyTEG (Mexico).

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