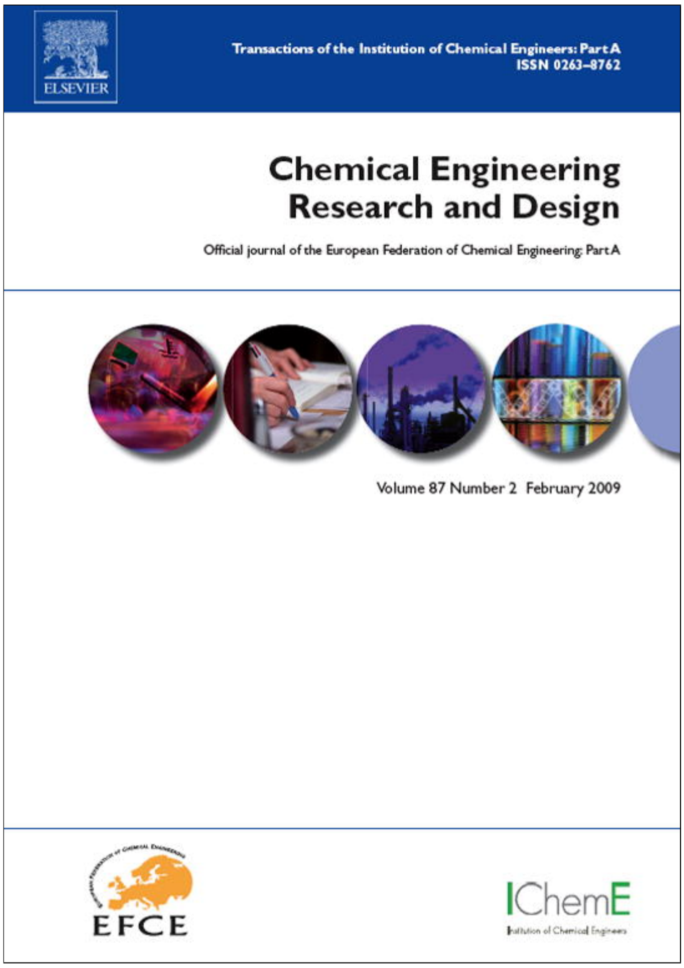

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Reducing energy consumption and CO_2 emissions in extractive distillation

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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 close boiling point mixtures and azeotropic mixtures using the two distillation sequences. Regarding energy consumption, total annual cost, thermodynamic efficiency, greenhouse gas emissions and theoretical control properties, the thermally coupled extractive distillation sequence outperformed the conventional extractive distillation sequence. The results showed that the energy savings predicted in the complex extractive distillation sequence can be achieved along with good operational properties and 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 CO_2 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 CO_2 emissions from distillation systems is an important issue, and much effort should be focused on energy savings techniques (Gadalla et al., 2005; Houghton, 2002). 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 (Rivero and Anaya, 1990). 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 CO_2 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 with equilibrium and nonequilibrium stage models (Triantafyllou and Smith, 1992; Annakou and Mizsey, 1996; Hernández and Jiménez, 1996, 1999; Dünnebier and Pantelides, 1999; Yeomans and Grossmann, 2000; Rev et al., 2001; Emtir et al., 2003; Olujic et al., 2003; Hernández et al., 2003, 2006; Hernández-Gaona et al., 2005; Abad-Zarate et al., 2006). These studies have shown that those thermally coupled distillation schemes are capable of typically achieving 30% energy savings over conventional schemes.

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Nomenclature

b	exergy function
G	transfer function matrix
h	molar enthalpy
n	mole flow
Q	reboiler heat duty
S	molar entropy
TAC	total annual cost
T_0	temperature of the surroundings
T_s	temperature of the system
W_{min}	minimum work for the separation
W_s	shaft work

Greek symbols

σ^*	maximum singular value
σ_*	minimum singular value
γ^*	condition number
η	second law efficiency

Extractive distillation is an important separation method in chemical engineering, and is used to separate compounds with similar boiling points or compounds that form azeotropes, by using an additional entrainer to alter relative volatility. Thus, it is possible to obtain one pure compound at the top of the column and the other, together with the entrainer component, at the bottom, which may be separated easily in a secondary distillation column, thanks to the high boiling point of the entrainer. Extractive distillation is widely used in several different processes: recovery of aromas or fragrances (Pollien et al., 1998; Chaintreau, 2001), separation of aqueous alcohol solutions (Pinto et al., 2000; Zhigang et al., 2002; Llano-Restrepo and Aguilar-Arias, 2003), mixtures which exhibit an azeotrope (Safrit and Westerberg, 1997; Rev et al., 2003; Xu and Wang, 2006; Wu et al., 2007) and separation of hydrocarbons with close boiling points (Liao et al., 2001; Lei et al., 2002; Wentink et al., 2007; Abushwireb et al., 2007).

The separation of azeotropic mixtures in batch distillation columns using entrainers has been also studied, for example, Lang et al. (1994) have studied the separation of a mixture of acetone and methanol using water as entrainer and they reported the use of an algorithm and a computer program to simulate the complex distillation process. Also, Low and Sorensen (2002) studied the optimal operation of the separation of the same azeotropic mixture, but they improved the distillation equipment using a middle vessel.

In this paper we study the purification of several different mixtures (only feasible the separations with extractive distillation) using the thermally coupled extractive distillation scheme with side rectifier (TCEDS-SR; Fig. 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 (Fig. 2) in terms of energy savings (reductions in greenhouse gas emissions), capital investment and control properties.

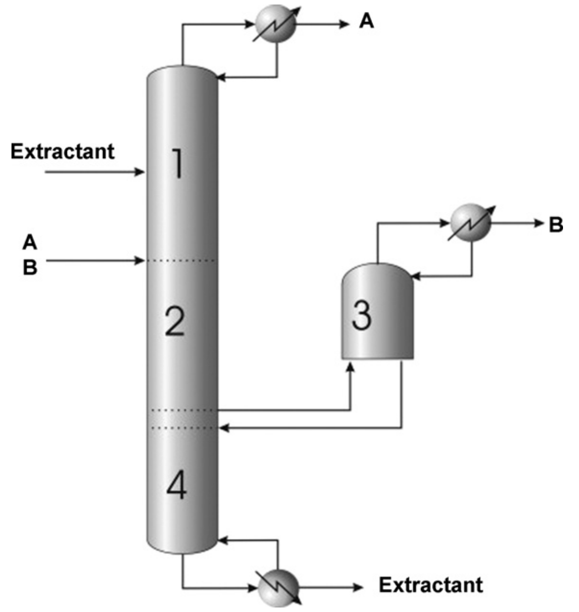

Fig. 1 – Thermally coupled extractive distillation sequence (TCEDS-SR).

It is important to highlight that this paper presents a new use of thermally coupled distillation sequences that have been used typically for the separation of hydrocarbon mixtures. The key difference between the previous use and this new application is the addition of a new feed (entrainer) to the main distillation column; as a result, the complexity of the optimization procedure is increased because two new search variables are introduced, i.e., the feed stage of the entrainer and the flowrate.

2. Design of extractive complex distillation schemes

In this paper, we present an energy-efficient design procedure for a thermally coupled extractive distillation scheme with side rectifier. 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 and (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. 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 (Figs. 1 and 2). After the tray arrangement

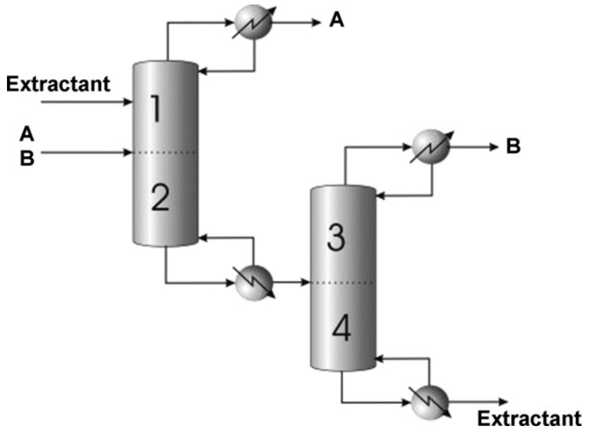

Fig. 2 – Conventional extractive distillation sequence (DS).

Table 1 – Mixtures analyzed

Mixture	Feed components	Feed component flows (kmol/h)	Extractant
M1 (azeotropic)	Tetrahydrofuran/water	40.82/4.53	1,2-Propanediol
M2 (azeotropic)	Acetone/methanol	45.35/45.35	Dimethyl sulfoxide (DMSO)
M3 (close boiling point)	*n*-Heptane/toluene	90.72/90.72	Aniline

for the TCEDS-SR sequence has been obtained, an optimization procedure is used to minimize the heat duty supplied to the reboilers 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^{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. This result implies that an optimum value has been detected for the design of the complex scheme. The search for the optimum design of the conventional distillation extractive scheme is conducted only on the extractant stream stage for the assumed value of the ratio of feed to extractant.

3. Thermodynamic efficiency

With the optimized designs of the TCEDS-SR schemes, thermodynamic efficiencies can be calculated using the laws of thermodynamics. For this task, we used the equations reported by Seader and Henley (1998), which are as follows:

- First law of thermodynamics:

$$\sum_{\text{out of system}} (nh + Q + W_s) - \sum_{\text{in to system}} (nh + Q + W_s) = 0 \quad (1)$$

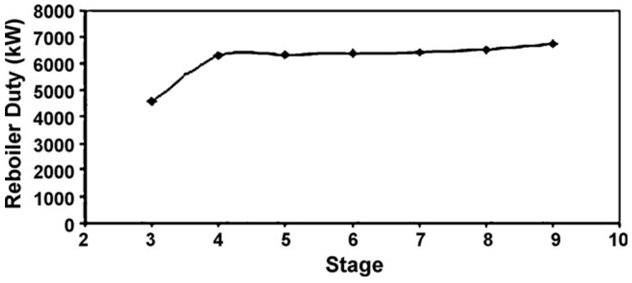

Fig. 3 – Optimization of the DS (case M2; E/F = 2.0).

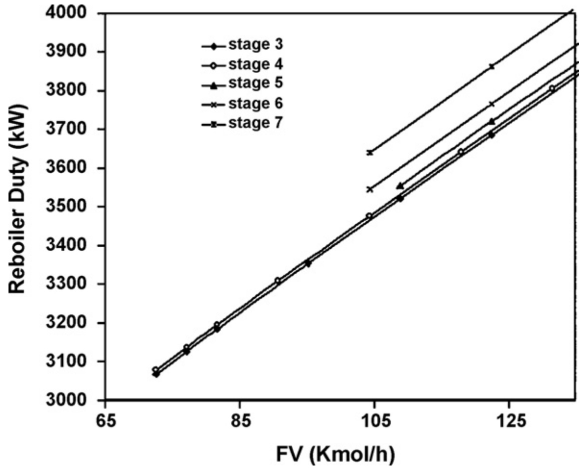

Fig. 4 – Search for energy-efficient design of the TCDES-SR (case M2; E/F = 2.0).

- Second law of thermodynamics:

$$\sum_{\text{out of system}} \left(ns + \frac{Q}{T_s}\right) - \sum_{\text{in to system}} \left(ns + \frac{Q}{T_s}\right) = \Delta S_{irr} \quad (2)$$

- Exergy balance:

$$\sum_{\text{in to system}} \left[nb + Q\left(1 - \frac{T_0}{T_S}\right) + W_s\right] - \sum_{\text{out of system}} \left[nb + Q\left(1 - \frac{T_0}{T_S}\right) + W_s\right] = LW \quad (3)$$

- Minimum work of separation:

$$W_{min} = \sum_{\text{out of system}} nb - \sum_{\text{in to system}} nb \quad (4)$$

- Second law efficiency:

$$\eta = \frac{W_{min}}{LW + W_{min}} \quad (5)$$

where $b = h - T_0$, s is the exergy function, $LW = T_0 \Delta S_{irr}$ is the lost work in the system and η is the thermodynamic efficiency. Thermodynamic properties such as enthalpies and entropies of the streams of the distillation sequences were evaluated through the use of a process simulator, Aspen Plus^{TM}.

4. Calculation of CO_2 emissions

In distillation systems, such as crude oil distillation units, carbon dioxide is generated mainly from furnaces, gas turbines, and boilers. These utility devices are the fuel consumers in refining plants and are used to provide heat, steam, and power to the process by burning a fuel. Therefore, these units are key drivers in energy savings oriented projects and for reducing

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 – Design variables for DS (M1; E/F = 2.0)

	Column 1	Column 2
Pressure (atm)	1.36	1
Stages	25	25
Feed stage	17	17
Extractant stage	3	

Table 4 – Design variables for TCEDS-SR (M2; E/F = 2.0)

	Main column	Side rectifier
Pressure (atm)	1.36	1.36
Stages	33	18
Feed stage	21	
Extractant stage	3	
Interconnection stage	30	
FV (kmol/h)	75.57	

environmental impact of emissions. Fuel is combusted when mixed with air, producing CO_2 according to the following stoichiometric equation:

$$C_xH_y + \left(x + \frac{y}{4}\right) O_2 \rightarrow xCO_2 + \frac{y}{2} H_2O \qquad (6)$$

where x and y denote the number of carbon, C, and hydrogen, H, atoms, respectively, present in the fuel compositions, and where complete oxidation of carbon is assumed.

In the combustion of fuels, air is assumed to be in excess to ensure complete combustion, so that no carbon monoxide is formed. CO_2 emissions, $[CO_2]_{Emiss}$ (kg/s), are related to the amount of fuel burnt, Q_{Fuel} (kW), in a heating device as follows (Gadalla et al., 2005):

$$[CO_2]_{Emiss} = \left(\frac{Q_{Fuel}}{NHV}\right)\left(\frac{C\%}{100}\right)\alpha \qquad (7)$$

where α (=3.67) is the ratio of molar masses of CO_2 and C, while NHV (kJ/kg) represents the net heating value of a fuel with a carbon content of C%.

Eq. (7) shows that both the fuel used and the heating device affect the amount of CO_2 produced.

Boilers produce steam from the combustion of fuel. This steam is delivered to the process at the temperature required by the process or obtained at a higher temperature and then throttled. In distillation systems, steam is used either for heating purposes, indirectly in reboilers, or as a direct stripping agent in so-called steam distillations, such as crude oil units.

Table 5 – Design variables for DS (M2; E/F = 2.0)

	Column 1	Column 2
Pressure (atm)	1.36	1
Stages	31	20
Feed stage	21	18
Extractant stage	3	

Table 6 – Design variables for TCEDS-SR (M3; E/F = 2.5)

	Main column	Side rectifier
Pressure (atm)	1.36	1.36
Stages	53	17
Feed stage	20	
Extractant stage	13	
Interconnection stage	39	
FV (kmol/h)	172.36	

The flame temperature is lower in a boiler than in a furnace because the heat of combustion is removed immediately to the steam. However, the same theoretical flame temperature of 1800 °C may still be used. The stack temperature of 160 °C is also used in the calculations. The amount of fuel burnt can be calculated from (Gadalla et al., 2005):

$$Q_{Fuel} = \frac{Q_{Proc}}{\lambda_{Proc}}(h_{Proc} - 419)\frac{T_{FTB} - T_0}{T_{FTB} - T_{Stack}} \qquad (8)$$

where λ_{Proc} (kJ/kg) and h_{Proc} (kJ/kg) are the latent heat and enthalpy of steam delivered to the process, respectively, while T_{FTB} (°C) is the flame temperature of the boiler flue gases. The above equation is obtained from a simple steam balance around the boiler to relate the amount of fuel necessary in the boiler to provide a heat duty of Q_{proc}; the boiler feed water is assumed to be at 100 °C with an enthalpy of 419 kJ/kg. Smith and Delaby (1991) provide a detailed derivation for Eq. (8) and state all employed basic assumptions. Eqs. (7) and (8) can be used to calculate CO_2 emissions from steam boilers.

5. Control properties

One of the basic and most important tools of modern numerical analysis is the singular value decomposition technique (SVD). There are numerous important applications of the SVD tool when quantitative and qualitative information is desired about a linear map. One important use of the SVD technique is in the study of theoretical control properties in chemical process. The definition of SVD implies:

$$G = V\Sigma W^H \qquad (9)$$

where G is the matrix where SVD is applied, $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, σ_i = singular value of $G = \lambda_i^{1/2}(GG^H)$; $V = (v_1, v_2, \ldots)$ matrix of left singular vectors, and $W = (w_1, w_2, \ldots)$ matrix of right singular vectors.

In the case where the SVD is used for the study of theoretical control properties, two parameters are of interest: the minimum singular value (σ_*) and the ratio maximum (σ^*) to minimum (σ_*) singular values or condition number (γ):

$$\gamma^* = \frac{\sigma^*}{\sigma_*} \qquad (10)$$

Minimum singular value is a measure of the invertibility of the system and represents a measure of the potential

Table 7 – Design variables for DS (M3; E/F = 2.5)

	Column 1	Column 2
Pressure (atm)	1.36	1
Stages	40	30
Feed stage	20	17
Extractant stage	13	

Table 8 – Results for different extractant/feed ratios, case M1

Sequence	Energy consumption (kW)	TAC ($/year)	η	CO_2 emissions (ton/h)
E/F = 2.0				
DS	2264.11	827624.71	48.40	0.62
TCEDS-SR	1719.49	656333.29	32.08	0.47
E/F = 2.5				
DS	2463.47	887466.55	27.95	0.68
TCEDS-SR	1823.18	686478.34	37.58	0.50
E/F = 3.0				
DS	2711.0	962586.56	30.20	0.74
TCEDS-SR	1943.06	721606.88	42.15	0.53
E/F = 3.5				
DS	2968.30	1040571.40	31.95	0.81
TCEDS-SR	2088.39	764676.89	45.62	0.57
E/F = 4.0				
DS	3228.83	1119517.07	33.39	0.89
TCEDS-SR	2243.70	810951.68	48.41	0.62

Table 9 – Results for different extractant/feed ratios, case M2

Sequence	Energy consumption (kW)	TAC ($/year)	η	CO_2 emissions (ton/h)
E/F = 2.0				
DS	5013.0	1503088.44	15.42	1.28
TCEDS-SR	2184.82	1101477.44	20.98	0.92
E/F = 2.5				
DS	5023.37	1629093.66	13.58	1.40
TCEDS-SR	2343.40	1136981.36	20.75	0.95
E/F = 3.0				
DS	5911.68	1748049.33	12.14	1.51
TCEDS-SR	3364.66	1193097.75	21.34	1.00
E/F = 3.5				
DS	6318.20	1959368.05	10.95	1.61
TCEDS-SR	3734.63	1306819.91	22.34	1.12
E/F = 4.0				
DS	6707.63	2073014.78	9.94	1.72
TCEDS-SR	3977.42	1381592.41	21.58	1.19

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 (Klema and Laub, 1980).

6. 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

Table 10 – Results for different extractant/feed ratios, case M3

Sequence	Energy consumption (kW)	TAC ($/year)	η	CO_2 emissions (ton/h)
E/F = 2.5				
DS	13552.88	4434047.19	18.56	3.9
TCEDS-SR	8508.84	2849003.61	31.67	2.93
E/F = 3.0				
DS	13648.51	4434955.68	17.23	3.93
TCEDS-SR	8769.68	2923992.68	17.31	2.62
E/F = 3.5				
DS	14025.70	4545937.63	16.25	4.03
TCEDS-SR	9246.85	3065257.31	18.83	2.76
E/F = 4.0				
DS	14495.43	4708939.80	16.13	4.16
TCEDS-SR	9795.05	3228368.09	19.02	2.93

describe 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. The pressure drop for a single tray is given based on the heuristics of Kister (1992). Purities of 99% in mole in the products were assumed.

7. Results

The resulting designs and their performance with respect to energy consumption, CO_2 emissions, thermodynamic efficiency, TAC and control properties are discussed in the following sections.

Design and energy optimization of the conventional and coupled sequence for each feed mixture were carried out using the procedure previously described. Typical optimization curves for the DS and TCEDS-SR (case M2) are shown in Figs. 3 and 4, 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 control design of this system appears to be an important task to be developed. Tray arrangements and some important design variables for that sequence after the optimization task are given in Tables 2–7.

The results of the rigorous optimization are collected in Tables 8–10 for the extractive distillation configurations, indicating the effect of solvent feed ratio (E/F) on energy consumption, economic evaluation, η and CO_2 emissions of the studied configurations. 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 (Triantafyllou and Smith, 1992). 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).

Table 11 – Minimum singular value and condition number for M1

E/F	Sequence	σ_*	γ
2.0	DS	1×10^{-7}	1.975×10^{10}
	TCEDS-SR	1×10^{-5}	1.386×10^{7}
2.5	DS	4×10^{-6}	6.514×10^{8}
	TCEDS-SR	9×10^{-5}	4.94×10^{8}
3.0	DS	9.8×10^{-5}	6.66×10^{8}
	TCEDS-SR	1×10^{-6}	1.074×10^{10}
3.5	DS	8.4×10^{-5}	3.2×10^{7}
	TCEDS-SR	1×10^{-6}	1.72×10^{9}
4.0	DS	1×10^{-8}	6.495×10^{17}
	TCEDS-SR	9.8×10^{-5}	2.937×10^{8}

Table 12 – Minimum singular value and condition number for M2

E/F	Sequence	σ_*	γ
2.0	DS	5.1×10^{-3}	12.5
	TCEDS-SR	8.06×10^{-2}	164.73
2.5	DS	3.4×10^{-3}	33.64
	TCEDS-SR	1.6×10^{-5}	3.857×10^{8}
3.0	DS	3×10^{-4}	1.647×10^{3}
	TCEDS-SR	1.3×10^{-5}	6.204×10^{8}
3.5	DS	6×10^{-3}	10.46
	TCEDS-SR	1.1×10^{-5}	5.03×10^{8}
4.0	DS	5.7×10^{-3}	10.92
	TCEDS-SR	1.09×10^{-5}	6.487×10^{8}

Table 13 – Minimum singular value and condition number for M3

E/F	Sequence	σ_*	γ
2.5	DS	2×10^{-5}	1.24×10^{4}
	TCEDS-SR	1×10^{-5}	6.77×10^{12}
3.0	DS	1×10^{-6}	4.089×10^{7}
	TCEDS-SR	1.45×10^{-5}	6.088×10^{12}
3.5	DS	1×10^{-7}	1.36×10^{8}
	TCEDS-SR	1.65×10^{-6}	2.592×10^{9}
4.0	DS	9.8×10^{-5}	2.674×10^{7}
	TCEDS-SR	1.44×10^{-6}	3.764×10^{7}

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 simulations were carried out in Aspen Dynamic^{TM} in order to obtain the transfer function matrix. Tables 11–13 provide the results for the SVD test for each sequence.

The TCEDS-SR option presents higher minimum singular values (at low values of E/F, in all cases of study); therefore, it can be expected that this coupled system will exhibit better control properties than the conventional extractive sequence under feedback control. The results for the condition number show that the complex sequence offers the best values at low E/F values. As a result, it can be expected that thermally coupled extractive distillation systems are better conditioned to the effect of disturbances than the conventional extractive arrangements.

In general, the control properties of TCEDS-SR options can be as good or better as those obtained in the conventional distillation sequences (at low values of E/F). However the best energy and TAC savings, η values and reduction of CO_2 emissions are better at high values of E/F.

8. 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. Regarding thermodynamic efficiency, in all cases, the introduction of thermal links increased its value (especially at high E/F values). Control properties have shown similarity to those of the conventional sequences (the integrated sequence presents similar or better minimum singular values and condition number in comparison to those obtained in the conventional distillation sequences for mixtures analyzed at low E/F values).

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; moreover, theoretical control properties indicate that energy savings and reduction and CO_2 emissions can be obtained without additional control properties, i.e., the expected dynamic behavior could be even better than that in the conventional extractive distillation sequence.

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Appendix A

For a given number of theoretical trays, Aspen Plus simulator calculates column diameter and height (for 24 in tray spacing) after converging for selected valve tray column with 2 in weir height. Valve trays of Glitsch type are used. The costing of distillation column (carbon steel construction) was estimated by the cost equations shown in Turton et al. (2004) that are updated with the CEPCI (Chemical Engineering Process Cost Index). For comparison, a single value of CEPCI is selected (October, 2007). The total column cost is the sum of the installed cost of column shell and the installed cost of column trays. Additionally, the sizing and costing of heat exchangers were calculated. The cost of heat exchangers can be correlated as a function of the surface area assuming shell and tube, floating head, and carbon steel construction. Installation prices are updated by the CEPCI index. Capital cost (purchase plus installation cost) is annualized over a period which is often referred to as plant life time:

$$\text{Annual capital cost} = \frac{\text{Capital cost}}{\text{Plant life time}} \tag{A.1}$$

$$\text{Total annual cost (TAC)} = \text{Annual operating cost} + \text{Annual capital cost} \tag{A.2}$$

Operating costs were assumed just utility cost (steam and cooling water).

Plant life = 5 years.

Operating hours = 8400 h/year.

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