

Energy Consumption in Sharp and Non-Sharp Splits of Ideal Ternary Mixtures

Sergi Expósito^a, Jordi Bone^{a,*}, Alexandra Elena Bonet-Ruiz^a, Joan Llorens^a, Petrica Iancu^b, Valentin Plesu^b

^aUniversity of Barcelona, Faculty of Chemistry, Department of Chemical Engineering and Analytical Chemistry, Martí i Franquès Street 1, 6th Floor, 08028 Barcelona, Spain

^bUniversity POLITEHNICA of Bucharest, Department of Chemical and Biochemical Engineering - Centre for Technology Transfer in the Process Industries, 1, Gh. POLIZU Street, Building A, Room A056, RO-011061 BUCHAREST, Romania
bonet@ub.edu

Most of the distillation processes deal with multicomponent mixtures, existing a great quantity of distillation sequences for this process. The sharp splits available for an ideal ternary mixture are the direct and the inverse distillation sequence scheme in which the compounds are separated in two different columns. There are non-sharp splits in which all the compounds are separated in a single distillation column that can incorporate a side column. Unfortunately, to choose non-sharp splits schemes, there is no heuristic that can provide information about the recommended cases, e.g. a single distillation column in which the intermediate boiling compound is collected by a side stream at the required purity or by other possibilities, such as the use of a side stripper or a side rectifier. The literature about this subject is very scarce, and many times when the non-sharp splits are used, no comparison with the sharp split alternatives is provided. Therefore, the cases for which the literature suggests the use of side columns are further studied, e.g. BTX (Benzene, Toluene, Xylene) mixtures separation. For many case studies, the results obtained show that the energy savings achieved, due to the use of side columns, are not significantly higher than the best sharp split process schemes. However, these results do not discard that for some other situations; the side column could be the most advantageous case.

Usually, it is considered that when the desired purity of the main product in a stream is reached, the impurities proportion do not affect significantly the energy consumption, and for most of the systems, this is true. However, for a mixture with a molar composition of 10 % isopentane, 10 % pentane and 80 % hexane (mol), when split in the respective compounds at a purity of 95 % (mol), very different energy requirements are depicted depending on the proportion of isopentane and hexane, present in the pentane stream obtained in a direct sequence process. The rigorous simulation results illustrate that almost 60% of the energy required to separate the above-mentioned mixture is saved when the pentane stream carries a mixture of isopentane and hexane. In addition, the environmental impact has been analyzed for each case studied, being reduced in the same way as the energy consumption does.

1. Introduction

Distillation, which is the separation technique used most in the chemical and petrochemical industry, is highly energy-intensive. Therefore, there has been an active search for means to reduce energy usage and costs (Malinen and Tanskanen, 2009). 90 % of all separation units and 5 % of the global energy demand can be attributed to distillation (Humphrey, 1995). This process is used to obtain different pure components of a mixture, although in some cases, to obtain more than one pure component is possible by the use of conventional sequences (direct or indirect distillation) or thermally-coupled columns processes, like the side-rectifier or the side-stripper distillation. Thermally-coupled columns offer a great opportunity to reduce energy consumption (Triantafyllou and Smith, 1992).

Usually, these columns are proposed directly as a better choice than direct or indirect sequences but many times, the results of non-conventional sequences are not compared with the conventional ones to confirm this

upgrade. Consequently, the energy consumption of sharp and non-sharp split processes for the mixtures proposed by Fang et al. (2017) and for BTX mixtures proposed by Kumar et al. (2017) have been analysed and compared to verify the use of non-conventional sequence processes.

Finally, the environmental impact has been analyzed for each process when using coal, oil or gas as fuel. Each one produces different components when its combustion reaction takes place, being the environmental impact lower or higher in the function of the compounds. For example, the combustion of coal produces particulate matter, various gases, mainly CO₂, CO, SO_x and NO_x droplets of organic compounds and trace elements, which are all released into the atmosphere, causing air pollution (Vamvuka, 1999).

The aim of the present study is to cover the lack of studies in the literature, to separate ternary mixtures are compared from an efficiency and environmental point of view using side strippers and rectifiers, versus the commonly used direct and indirect distillation sequences.

2. Methodology

Firstly, the energy efficiency of all the distillation sequences studied on this work has been analyzed by the DSE method (Distillation Sequence Efficiency), it is considered to be a resembled of the distillation column to a Carnot machine with the objective of obtaining an approximation of the aforementioned efficiency. Due to this estimation, it is possible to calculate the energy efficiency of the column developing properly for each case the Equation 1.

$$DSE = \sum x_i \cdot \prod \eta_{ic} \quad (1)$$

Where the compositions "x_i" are fixed by the feed and η_{ic} is the Carnot efficiency of the distillation column *i*, which has been calculated using the equation:

$$\eta_{ic} = \frac{T_{\text{hot source}} - T_{\text{cold source}}}{T_{\text{hot source}}} \quad (2)$$

When applying this formula to distillation columns, the hot source is always the temperature of the residue stream and the cold source is the temperature of the distillate stream.

Secondly, direct and indirect distillation sequence for each mixture considered is simulated rigorously using Aspen®Plus. For the simulation of the aromatic hydrocarbons' distillation and the BTX process, the initial composition, flow and pressure are fixed and specified on both of the articles studied. 'RadFrac' block has been used for the rigorous simulation, designed with a huge amount of distillation plates to achieve the equilibrium to make feasible the compounds split. Distillate flowrate has been used as a design specification to achieve a 95% purity of each compound varying the reflux ratio. Despite the fact that standard convergence is set by default, strongly non-ideal liquid convergence type has been selected to improve. Once the results of the simulation have been obtained, the distillation process is optimized, varying the impurities composition of the product streams to minimize the total energy consumption of the distillation column.

Finally, environmental impact has been analyzed for each process using the WAR (WAste Reduction Algorithm) software developed by the United States Environmental Protection Agency (EPA, 2019).

3. Results

For sharp and non-sharp splits of both processes (Fang et al. (2017) and Kumar et al. (2017)) used as case studies in order to analyze the efficiency of each distillation scheme process for its subsequent comparison and selection of the best sequence, DSE has been calculated. The DSE assessment was performed for process configurations involving Side Rectifier (SR), Side Stripper (SS), Direct Sequence (DS) and Indirect Sequence (IS).

Analyzing the DSE results of each distillation sequence, the use of the non-sharp splits is not justified due to the minimum improvement of the efficiency and harder control of the process (Table 1 and 2). Due to this fact, only sharp-split schemes (direct and indirect distillation) have been rigorously simulated. However, once the direct and indirect distillation have been simulated, the energy consumption of the non-sharp splits proposed in the articles have been compared with the one obtained by simulation in order to prove the veracity of the results obtained using the DSE method.

Table 1: DSE values (dimensionless units) for mixtures (Fang et al., 2017)

Compound	Composition (% mol)	DSE SR	DSE SS	DSE DS	DSE IS
n-C ₅ H ₁₂	10.00				
n-C ₆ H ₁₄	10.00	0.824	0.829	0.823	0.812
n-C ₇ H ₁₆	80.00				
Benzene	10.00				
Toluene	10.00	0.823	0.832	0.822	0.810
Ethylbenzene	80.00				
i-C ₅ H ₁₂	10.00				
n-C ₅ H ₁₂	10.00	0.821	0.814	0.820	0.811
n-C ₆ H ₁₄	80.00				

Table 2: DSE values (dimensionless units) for the BTX mixtures proposed by Kumar et al (2017) using Side Rectifier (SR), Side Stripper (SS), Direct Sequence (DS) and Indirect Sequence (IS)

Compound	Composition (% mol)	DSE SR	DSE SS	DSE DS	DSE IS
Benzene	60.00				
Toluene	20.00	0.308	0.319	0.280	0.234
Xylene	20.00				
Benzene	20.00				
Toluene	60.00	0.278	0.282	0.266	0.263
Xylene	20.00				
Benzene	20.00				
Toluene	20.00	0.646	0.650	0.641	0.626
Xylene	60.00				
Benzene	12.54				
Toluene	39.31	0.532	0.534	0.527	0.522
Xylene	48.15				
Benzene	60.18				
Toluene	23.29	0.276	0.287	0.245	0.204
Xylene	16.53				

Direct and indirect distillation sequences have been simulated using Aspen®Plus to obtain a value of the minimum energy consumption of the process. Furthermore, once the process has been simulated, it is optimized, reducing the energy needed by varying the composition of the impurities (Table 3).

Table 3: Energy consumption of the direct distillation sequence for mixtures (Fang et al., 2017)

Compound	Composition (% mol)	Q _{reb.} DS optimized (kW)	Q _{reb.} DS (kW)	Energy improvement (%)
n-C ₅ H ₁₂	10.00			
n-C ₆ H ₁₄	10.00	29.00	29.21	0.68
n-C ₇ H ₁₆	80.00			
Benzene	10.00			
Toluene	10.00	39.12	44.11	11.33
Ethylbenzene	80.00			
i-C ₅ H ₁₂	10.00			
n-C ₅ H ₁₂	10.00	41.84	103.03	59.39
n-C ₆ H ₁₄	80.00			

Results obtained indicate a very important improvement for a 10 % isopentane, 10 % n-pentane and 80 % n-hexane mixture (mol) when the process is optimized by its impurities composition of almost a 60 % of energy-saving (Table 3). That important improvement is due to the proximity of the boiling point between the i-pentane (27.8 °C) and the n-pentane (36.1 °C), and the relative volatility is nearly the unit, being a difficult separation by distillation. Optimizing the process, it is possible to vary the impurities composition to reduce the energy consumption, due to the difficult separation in some cases these impurities compositions have direct and important effects upon the energy consumption. Furthermore, it is also possible to reduce over an 11 % the consumption by varying the impurities composition when distilling a 10 % benzene, 10 % toluene and 80 % ethylbenzene mixture (mol) by direct sequence.

Table 4: Energy consumption of the indirect distillation sequence (IS) for mixtures (Fang et al., 2017)

Compound	Composition (% mol)	Q _{reb.} IS optimized (kW)	Q _{reb.} IS (kW)	Energy improvement (%)
n-C ₅ H ₁₂	10.00			
n-C ₆ H ₁₄	10.00	24.60	26.00	5.40
n-C ₇ H ₁₆	80.00			
Benzene	10.00			
Toluene	10.00	30.50	30.55	0.07
Ethylbenzene	80.00			
i-C ₅ H ₁₂	10.00			
n-C ₅ H ₁₂	10.00	32.20	32.60	1.23
n-C ₆ H ₁₄	80.00			

Optimizing the indirect distillation for a 10 % n-pentane, 10 % n-hexane and 80 % n-heptane mixture, to reduce over a 5 % the energy consumption of the process (Table 4) is possible, being an improvement to be considered when designing the process.

Table 5: Energy consumption of the direct distillation sequence (DS) for mixtures (Kumar et al., 2017)

Compound	Composition (% mol)	Q _{reb.} DS optimized (kW)	Q _{reb.} DS (kW)	Energy improvement (%)
Benzene	20.00			
Toluene	60.00	3,781.4	3,962.4	4.6
Xylene	20.00			
Benzene	12.54			
Toluene	39.31	3,256.4	3,359.0	3.0
Xylene	48.15			

Table 6: Energy consumption of the indirect distillation sequence (IS) for mixtures (Kumar et al., 2017)

Compound	Composition (% mol)	Q _{reb.} IS optimized (kW)	Q _{reb.} IS (kW)	Energy improvement (%)
Benzene	60.00			
Toluene	20.00	4,332.8	4,419.9	2.0
Xylene	20.00			
Benzene	20.00			
Toluene	60.00	4,087.4	4,393.3	6.9
Xylene	20.00			
Benzene	60.18			
Toluene	23.29	4,469.8	4,571.0	2.2
Xylene	16.53			

For the distillation of the BTX mixtures, when the impurities are optimized in the direct (Table 5), and indirect (Table 6) distillation sequence is possible to improve the process reducing the energy consumption in most of the cases analyzed. Almost 7 % of energy consumption reduction is reached for a 20 % benzene, 60 % toluene and 20 % xylene mixture (mol) when its separation by indirect sequence is optimized. Furthermore, for the previously mentioned same mixture and composition, using the direct distillation sequence, a 4.6 % reduction of energy consumption can be achieved. Other BTX mixtures of Kumar et al. (2017) have been simulated but reaching improvement under 1 %, hence these cases have not been considered as an important improvement. Comparing the energy consumption results of the non-sharp splits proposed on both articles, the DSE values are validated as the energy consumption of the sharp splits (direct and indirect sequence) is, in most cases, very similar to the consumption of the intensified distillation process in the articles analyzed. Once the simulation, optimization and subsequent comparison of the process have been done, the environmental impact has been analyzed by using EPA WAR® software (Table 7 and 8). the relation between the reduction of energy consumption due to the optimization of the process and the reduction of its environmental impact has been verified. Therefore, environmental impact has been improved similarly to the energy consumption optimization, i.e. the following results correspond to the environmental impact from the direct distillation sequence of the aromatic hydrocarbons mixture proposed on Fang et al. (2017) when optimized by the impurities composition *i* (Table 8) and without optimization (Table 7).

Table 7: Potential Environmental Impact (PEI) for the direct distillation sequence (Fang et al., 2017)

Inlet Flow (mol/s)		DIRECT SEQUENCE				
Compound	Composition (% mol)	Inlet (kg/h)	Energy usage (MJ/h)	Type of fuel		
				Coal	Gas	Oil
				I_{out} (PEI/kg)	I_{out} (PEI/kg)	I_{out} (PEI/kg)
n-C ₅ H ₁₂	10.00					
n-C ₆ H ₁₄	10.00	345.6	105.3	$2.01 \cdot 10^{-3}$	$3.37 \cdot 10^{-4}$	$1.31 \cdot 10^{-3}$
n-C ₇ H ₁₆	80.00					
Benzene	10.00					
Toluene	10.00	367.1	158.7	$2.85 \cdot 10^{-3}$	$4.78 \cdot 10^{-4}$	$1.86 \cdot 10^{-3}$
Ethylbenzene	80.00					
i-C ₅ H ₁₂	10.00					
n-C ₅ H ₁₂	10.00	300.1	370.7	$8.15 \cdot 10^{-3}$	$1.36 \cdot 10^{-3}$	$5.31 \cdot 10^{-3}$
n-C ₆ H ₁₄	80.00					

Table 8: Potential Environmental Impact (PEI) for the optimized direct distillation sequence (Fang et al., 2017)

Inlet Flow (mol/s)		OPTIMIZED DIRECT SEQUENCE				
Compound	Composition (% mol)	Inlet (kg/h)	Energy usage (MJ/h)	Type of fuel		
				Coal	Gas	Oil
				I_{out} (PEI/kg)	I_{out} (PEI/kg)	I_{out} (PEI/kg)
n-C ₅ H ₁₂	10.00					
n-C ₆ H ₁₄	10.00	345.6	104.3	$1.99 \cdot 10^{-3}$	$3.33 \cdot 10^{-4}$	$1.30 \cdot 10^{-3}$
n-C ₇ H ₁₆	80.00					
Benzene	10.00					
Toluene	10.00	367.1	140.6	$2.53 \cdot 10^{-3}$	$4.23 \cdot 10^{-4}$	$1.65 \cdot 10^{-3}$
Ethylbenzene	80.00					
i-C ₅ H ₁₂	10.00					
n-C ₅ H ₁₂	10.00	300.1	150.6	$3.31 \cdot 10^{-3}$	$5.54 \cdot 10^{-4}$	$2.16 \cdot 10^{-3}$
n-C ₆ H ₁₄	80.00					

For the direct sequence distillation of a mixture with a molar percentage of 10 % i-pentane, 10 % n-pentane and 80 % n-hexane, the environmental impact is reduced nearly 60 % when optimized by the impurities composition, the same improvement as the energy consumption reduction. Results for the indirect sequence for these aromatics hydrocarbons and the distillation process of different BTX mixtures proposed on Kumar et al. (2017) prove the direct relation between the energy consumption and the environmental impact. An improvement has been achieved from the environmental impact as well as the process is energetically optimized, being both reduced.

4. Conclusions

When sharp splits and non-sharp splits of both articles studied have been analyzed by the DSE method, it has been observed the similarity on their efficiency values. Therefore, once the comparison has been done, it is possible to conclude that the use of non-sharp splits (side rectifier and side stripper distillation) is not justified, at least energetically.

Energy consumption of the process has been reduced when distilling by conventional sequences in most of the different mixtures studied optimizing the process varying the composition of its impurities. Important improvements have been achieved by this optimization method, reaching energy savings up to 11 % for a BTX mixture 10 %, 10 % and 80 % (%mol) respectively, and almost a 60 % for a 10 % i-pentane, 10 % n-pentane and 80 % n-hexane (% mol) mixture. Furthermore, environmental impact has been analyzed for each case studied verifying the relation between that impact and the energy consumption of the process. Consequently, the environmental impact has been reduced to the same extent as the energy consumption when the process has been optimized, and gas fuel is less polluting.

Finally, the energy consumption of the intensified columns, proposed on both articles, has been compared with the consumption of the non-intensified columns simulated on this article. As predicted by the DSE method, the energy consumption between the intensified and non-intensified columns is closely equal, remarking the importance to take into account conventional direct and inverse sequences when side strippers or rectifiers are proposed.

Acknowledgements

The authors would like to thank the financial support of the project CTM2016-76275-R (Ministry of Economy, Industry and Competitiveness –Spanish Government) who provided the opportunity to complete this research. Two authors (VP and PI) are grateful for the financial support received in the framework of structural project POC P_37_449 contract 155/25.11.2016, code MySMIS 107714.

References

- EPA, 2019, Waste Reduction Algorithm, <epa.gov/chemical-research/waste-reduction-algorithm-chemical-process-simulation-waste-reduction>, accessed 05.03.2019.
- Fang T., Ye Y., Xigang Y., Yiqing L., 2017. Influence of mixture and separation requirements on optimal configuration for ternary distillation. *Huagong Xuebao/CIESC Journal*, 68(2), 708-715.
- Humphrey L., 1995. Separation processes: playing a critical role. *Chem. Eng. Prog.*, 91(10), 31–32.
- Kumar S., Gupta S., Nanoti S.M., 2017. Techno-economic evaluation of top, middle, and bottom divided wall column configurations for benzene, toluene, and xylene processing in aromatic production plant, *Separation Science and Technology*, 52(1), 122-131.
- Malinen I., Tanskanen J., 2009. Thermally coupled side-column configurations enabling distillation boundary. *Ind. Eng. Chem.*, 48, 6387-6404.
- Triantafyllou C., Smith R., 1992. The design and optimisation of fully thermally coupled distillation columns. *Chem Eng Res Des*, 70(A2), 118-132.
- Vamvuka D., 1999. Environmental Impacts of Coal Utilization on the Ecosystem. *Energy Exploration & Exploitation*, 17(6), 583–605.