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A Stepwise Framework for Flowsheet Integration in Extractive Distillation

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The aim of this work is to develop a stepwise framework for energy saving in extractive distillation process on the view of flowsheet integration. It combines process simulation, heat integration and heuristic rule. Evolutionary approach is applied for flowsheet integration according to heuristic rules. C-5 mixture separation process with acetonitrile (ACN) as the solvent is presented as a case study. Based on the heat integration and heuristic rules, an optimal integrated flowsheet was obtained. The simulation results showed that the total consumption of utility could save up to 39.3% compared with the conventional flowsheet before heat integration and 12.5% after heat integration.

1. Introduction

Extractive distillation is the common separation method for separating azeotropes and mixtures of components having close boiling point in the petrochemical industry. And this process is energy-intensive. Motivated by energy and capital savings, some methodologies and techniques have been reported. Li et al. proposed energy-saving approach using intermediate reboiler and thermally coupled distillation (Li *et al,* 2002). Lei et al. discussed process design for separating C-4 mixtures using extractive distillation (Lei *et al*., 2003). Meyer et al. proposed coupled distillation to treat C-4 fraction (Meyer *et al.*, 2003). Literature examples show that heat integration can make a great improvement from a systematic perspective. Focusing on heat integration, considerable research efforts have been made to develop systematic methods. Examples include pinch technology, heuristics, and mathematic programming (Zhu *et al*., 2000; Smith, 2005; Klemes *et al*., 2006).

The aim of this work is to develop a stepwise framework for energy saving in extractive distillation process. This article is organized as follows. Initially, the methodology for extractive distillation is proposed. The focus is on the evolutionary approach and heuristic rules. Then the proposed framework is demonstrated for the C-5 mixture separation process. Three flowsheet schemes are explored and compared. Finally, conclusions are presented.

2. Methodology

2.1 The framework and heuristic rules

For a given mixture of extractive distillation, a conventional process (base case) is designed. Based on the base case, heat integration is implemented using the heat flow match. Then complex columns are introduced in the heat-integrated scheme according to heuristic rules, and the flowsheet-integrated scheme is generated. Finally, heat integration for the flowsheet-integrated scheme is implemented. Fig. 1 shows the conceptual diagram for the stepwise framework.

We proposed six heuristic rules for extractive distillation. They related to the phase state of feed, the number of reboiler, side-draw distillation, solvent, etc.

Rule 1: The vapor feed is preferred.

Rule 2: The reduction of the number of solvent column is preferred.

Rule 3: The reduction of the liquid flow rate of stripping section in each column is preferred. It leads to increase the efficiency of column.

Rule 4: The side-draw is preferred.

Rule 5: The reduction of the number of reboilers is preferred. It leads to reduce the energy consumption and equipment investment.

Rule 6: The match of heat flows in plant-wide is preferred.

2.2 Evolutionary approach

According to the stepwise framework, the detailed procedure of implementation is presented. It is an evolutionary process as shown in Fig. 2. The procedure is following as:

(1) The separation problem is specified;

(2) The conventional flowsheet is generated according to industrial and engineering experience;

(3) The flowsheet is simulated with the simulator;

(4) The heat flows of the flowsheet are analyzed and the heat integration is determined;

(5) The objective function value is calculated. The economic objective function is the sum of costs of cooling water and steam. If satisfying the requirements, jump to step (7). If not, go on to step (6); The requirements should be satisfied in separation process, such as rate of product recovery, product purity, pressure, temperature, stage number, safety, etc

(6) The flowsheet scheme is modified with heuristic rules, and the new scheme possessing the complex columns is generated, return to step (3);

(7) The final flowsheet is determined after comparing the schemes.

3. Case study

3.1 Process statements

Fig. 3(a) shows the C-5 mixture separation process extracting isoprene as the primary product from petroleum hydrocarbon mixtures. This process consists of six columns. The solvent is acetonitrile (ACN). The feed mixture contains eight components as listed in Table 1. Pure isoprene (99.5 wt % or more) is obtained as the bottom product D5. The detailed operation parameters of this process are provided in the thesis (Yu, 2006).

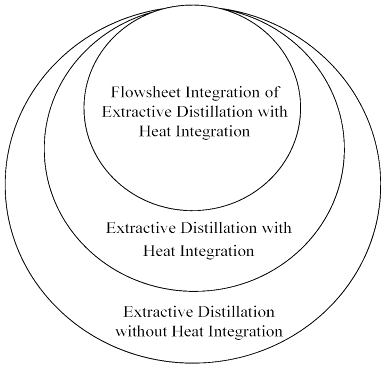


Fig. 1 Stepwise framework for solving flowsheet integration of extractive distillation

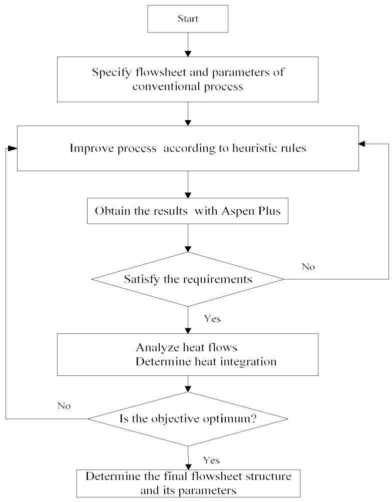


Fig. 2 Evolutionary approach for flowsheet integration of extractive distillation

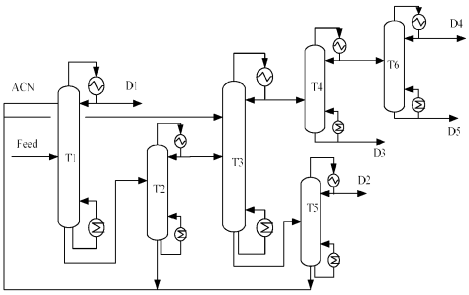
Table 1 Data for each component of feed mixture

Components	Flowsheet rate kg/h	Boiling point ℃	Relative Volatility α (without ACN)	Relative Volatility α (with 75% ACN)
n-pentane	200.00	36.07	0.935	2.37
cis-2-Pentene	10.00	36.94	0.913	1.49
trans-2-Pentene	200.00	36.35	0.931	1.56
isoprene	20.00	34.07	1.000	1.00
1,4-pentadlene	20.00	25.97	1.295	—
cyclopentene	40.00	44.24	0.719	—
1,3-cyclopentadiene	30.00	42.50	0.811	0.62
1-pentyne	3.00	40.18	0.839	0.58

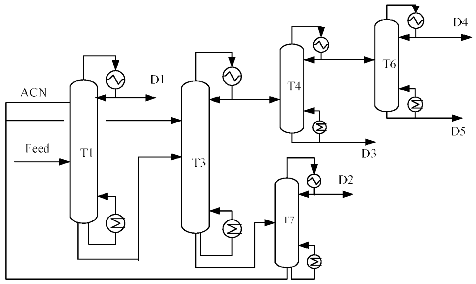
3.2 Evolutionary approach

According to the proposed evolutionary approach, we obtain three flowsheet schemes as shown in Fig. 3 (b ~ d). From conventional flowsheet to scheme 3, it is an evolutionary process. As the example, the evolutionary process from scheme 2 to scheme 3 is presented as followed.

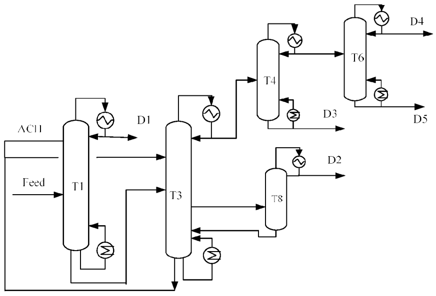
Fig. 4 showed the total vapor and liquid flow rates in T1 and T3 of scheme 2 without heat integration. The results show high liquid flow rates led to high heat duty of the bottom in T1 and T3. Moreover, the thermal coupling distillation is not easy to control. Therefore, according to heuristic rule 3 and 4, scheme 3 is generated. A vapor stream is withdrawn from T1 and fed into T3. A vapor stream is withdrawn from the pentyne-rich stage in T3 and fed into T9. The modified scheme is shown as Fig. 3 (d). Fig. 5 showed the total vapor and liquid flow rates in T1 and T3 of scheme 3 without heat integration. Compared scheme 2, the total vapor and liquid flow rates are decreased distinctly.



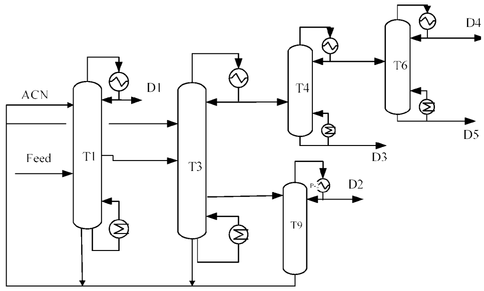
(a) Conventional flowsheet



(b) Flowsheet of evolutionary scheme 1



(c) Flowsheet of evolutionary scheme 2



(d) Flowsheet of evolutionary scheme 3

Fig. 3 Conventional flowsheet and Flowsheet schemes according to evolutionary approach
(T1- extraction column #1, T2- solvent recovery #1, T3- extraction column #2,
T4- removing heavy components, T5- solvent recovery #2, T6- removing heavy components,
T7- solvent separator, T8-removing 1-pentyne, T9- water scrubbing column)

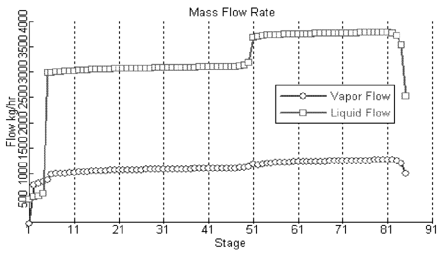


Fig. 4 (a) Stagewise variation of vapor & liquid flow rates in T1 (scheme 2)

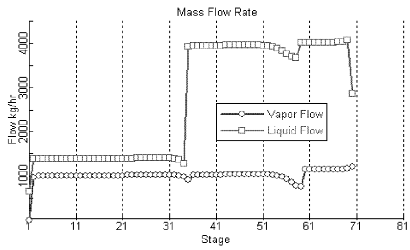


Fig. 4 (b) Stagewise variation of vapor & liquid flow rates in T3 (scheme 2)

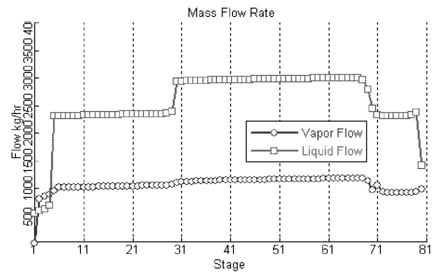


Fig. 5 (a) Stagewise variation of vapor & liquid flow rates in T1 (scheme 3)

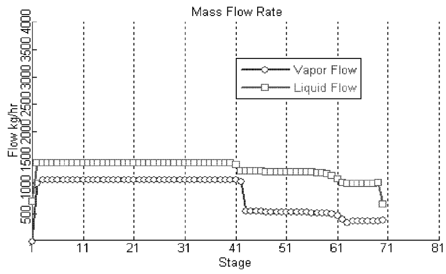


Fig. 5 (b) Stagewise variation of vapor & liquid flow rates in T3 (scheme 3)

According to scheme 3, heat integration can be implemented. The heat cascade use (among T1, T3 and T4) and steam consumption are:

(1) heat cascade use of T1 bottom flow

The reboiler of T4 68.78 °C intermediate reboiler of T6 60.00°C

114.53°C. ----------------------------> 80.00°C ----------------------------> 70.00°C

$Q=52.41\times10^3$ kcal/h $Q=17.47\times10^3$ kcal/h

(2) heat cascade use of T3 bottom flow

The reboiler of T4 68.78°C intermediate reboiler of T6 60.00°C

102.40°C. ----------------------------> 80.00°C ----------------------------> 70.00°C

$Q=15.05\times10^3$ kcal/h $Q=6.84\times10^3$ kcal/h

(3) consumption of steam

T1 reboiler 114.53 °C

150.0°C. ----------------------------> 150.0°C

$Q=200.07\times10^3$ kcal/h

T3 reboiler 102.40 °C

150.0°C. ----------------------------> 150.0°C

$Q=70.51\times10^3$ kcal/h

T4 reboiler 68.78 °C

150.0°C. ----------------------------> 150.0°C

$Q=126.76\times10^3$ kcal/h

where Q is the heat to exchange.
The utility consumption for scheme 3 is calculated as shown in Table 2.

Table 2 Utility consumption before & after heat integration for scheme 3

	Steam (t/t)	Cooling water (t/t)
Before Heat Integration	6.026	262.602
After Heat Integration	4.087	262.602
Decrease (%)	32.17	0

3.3 Results

The four schemes are compared according to the number of columns and utility cost as shown in Table 3. The performance of scheme 3 is better than the remaining. The simulation results showed that the total consumption of utility of Scheme 3 could save up to 39.3% compared with the conventional flowsheet before heat integration and 12.5% after heat integration.

Table 3 Comparison of each scheme

		conventional	Scheme 1	Scheme 2	Scheme 3
Number of Columns		6	5	5	5
Total cost of Utility*	Before Heat Integration ($/t)	74.7	69.9	65.4	58.5
	After Heat Integration ($/t)	51.8	48.5	50.3.	45.3

* Assume that costs of cooling water (28) and steam (150℃, $1kg/cm^2$) are 0.067$/t and 6.8$/t.

4. Conclusion

This article presents a stepwise framework for saving energy of extractive distillation. Evolutionary approach is introduced to generate new flowsheet schemes based on heat integration and heuristic rules. C-5 mixture separation process is used to demonstrate the framework. The detailed steps of flowsheet integration are implemented. Compared the schemes, an optimal integrated flowsheet was obtained.

5. References

Klemes J., P. Stehlk, 2006, Recent advances on heat, chemical and process integration, multi-objective and structural optimization, Applied Thermal Engineering 26 (13):1339 – 1344.

LEI Z., B. CHEN, J. LI, 2003, Process Design for Separating C4 Mixtures by Extractive Distillation, Chinese Journal of Chemical Engineering, 11(3): 297-301.

LI Y., X. FAN, P. YAO, 2002, Energy and water saving of extracting butadiene process by extractive distillation, Modern Chemical Industry, 22: s143-152 (in Chinese)

Meyer G., K. Gerd, B. Gerd, et al.,2003, Method and device for treating a C4 fraction, US, patent, A1 0181772, 2003/09/25

Smith R., 2005, Chemical Process Design and Integration, John Wiley&-Sons, Ltd, Chichester, England.

Yu H., 2006, Strategy study of saving energy in extractive distillation flowsheet integration. Master thesis. Qingdao University of Science & Technology (in Chinese)

Zhu X., L. Vaideeswaran, 2000, Integration in Analysis and Optimization of Energy Systems. Applied Thermal Engineering, 20: 1381-1392