Simultaneous heat integration and parameter optimization for thermally coupled complex distillation flowsheet

Dong Fenglian, Yuan Xigang, Luo Yiqing

State key laboratory of Chemical Engineering (Tianjin University), Chemical Engineering Research Center, Tianjin University, Tianjin 300072, China, yuanxg@tju.edu.cn

Abstract: This paper addresses the problem of simultaneous heat integration and parameter optimization for a given complex distillation column flowsheet. A general design procedure including converting a complex distillation column flowsheet into its thermodynamic equivalent simple column sequence, the shortcut design of the equivalent sequence, and heat integration structure generation with pinch design method is developed. The example demonstrated that the design procedure can give effectively all the needed design parameters and heat integration structure.

Keywords: thermally coupled complex distillation flowsheet; simultaneous heat integration and parameter optimization; pinch design method

1. Introduction

Distillation is a widely used separation process and it is the largest energy consumer among process unit operations in process industries. For multicomponent separation, the heat integrated complex distillation schemes are very promising alternatives for both energy and capital savings. However, the problems of optimal synthesis of heat integrated complex distillation flowsheets are complex, and the research on investigating and developing powerful methods to solve such problems remains open. Heat integration and parameter optimization for a given flowsheet structure of complex distillation columns is

still challenging, especially for those including fully thermally coupled columns where the spread ratio for the key components in the pre-fractionators, reflux ratios and operating pressures of the columns, as well as the heat integrated structure need to be simultaneously optimized.

In this paper, the problem of simultaneous heat integration and parameter optimization for a given complex distillation column flowsheet is addressed. The design results can be used as the initial information for rigorous simulation and to compare among the feasible alternatives so that the optimal configuration can be obtained.

2. Problem Statement

The problem addressed in this paper can be stated as follows:

A single feed stream of N-component mixture of known conditions (i.e. composition, flow rate, temperature and pressure) is given. For a given complex distillation flwosheet structure of separating the mixture into (relative) pure component, the problem is to find out the optimal operation parameters and heat integration structure that make the total annual cost minimum.

The complex distillation flowsheet considered here can involve simple columns, complex columns with intermediate side-draws and corresponding side strippers or side rectifiers, partially and/or fully thermally coupled columns with prefractionators. Heat integration between condensers and reboilers of various columns are allowed.

To reduce the complexity of the synthesis problem, we make the following assumptions:

   (1) The mixture to be separated doesn't form azetropes.

   (2) All the vapor streams are saturated vapor and all the liquid streams are saturated liquid.

   (3) Only one middle component exists between a prefractionator's light and heavy key component.

The first two assumptions have been widely adopted for the synthesis of distillation systems. Assumption (3) is just for reducing the problem's complexity. If there is more than one component between the light and heavy key component in the prefractionator, the problem's complexity will increase very largely and the evaluation for such a situation will be much more complicated.

3. Solution Strategies

3.1. Thermodynamic equivalent scheme for complex distillation flowsheet

A complex distillation flowsheet can be converted into its thermodynamic equivalent simple column flowsheet[1-3]. For example, a distillation flowsheet
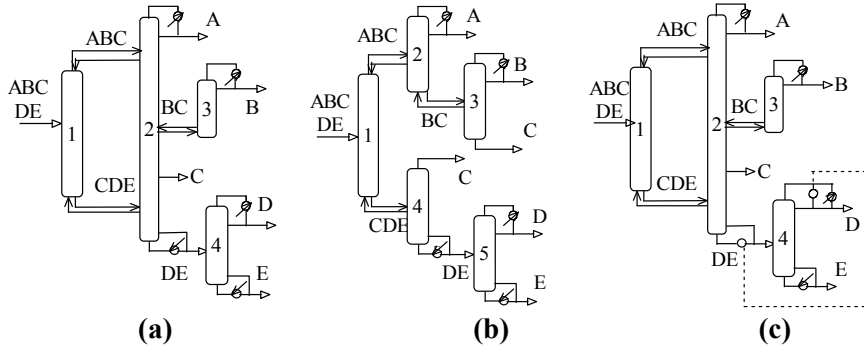
Figure 1 Complex distillation flowshee and its equivalent flowsheet
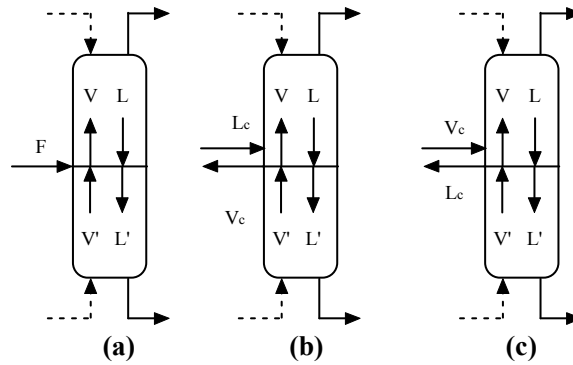

Figure 2 Three basic units of thermodynamic equivalent schemes

for the separation of a five component mixture shown in Fig.1a can be converted into its thermodynamic equivalent configuration of simple columns as shown in Fig.1b. Note that the number of column sections and heat exchangers in two configurations are the same. Each unit column in the equivalent configuration can be considered as a simple column with one stripping section and one rectifying sections. The equivalent configuration has the following properties.

 (1) The feed to a column may have one of the three possible states: a saturated liquid（Fig.2a）, or one of the two types of thermally coupling streams shown in Fig.2b and Fig.2c.

(2) Columns linked with thermally coupling streams should have the same operating pressure. For example, in Figure.1b, column 1, 2 , 3 and 4 should have the same operation pressure. Also if one column's bottom product component is same with another's top product component, they should have the same operating pressure, because in the complex flowsheet they belong to one column. For example, in Fig1.b, column 3 and 4 should have the same pressure. Moreover, if one column's bottom product component is same with another's top product component, the first column's stripping section's vapor flow rate
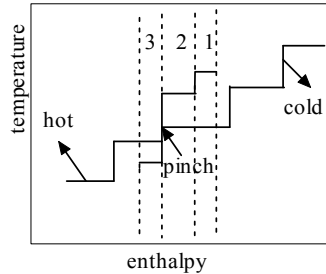
Fig 3 Composite curves for heat integration

should be the same with the second column's rectifying section's vapor flow rate.

3.2. The shortcut method of designing the thermodynamic equivalent simple columns

The shortcut method based on Fenske_Underwood_Gilliland[1-3] is applied for designing the thermodynamic equivalent simple columns. According to the shortcut method, when the columns' operating pressures p, operating reflux ratios r, the light key components' recovery ξ_{LK} , heavy key components' recovery ξ_{HK} of the prefractionators and flowrates and compositons for all the streams (material balance) are specified, all design parameters such as theoretical and real trays, the minimum reflux *etc*. can be calculated. After these parameters are obtained, the columns' top temperatures and bottom temperatures T, the condensers' heat duty Q_c and reboilers' heat duty Q_r are determined.

3.3. Design of the heat exchange network with the pinch design method

After the temperatures and heat duty of all the streams are determined, the next question is to determine the optimal heat exchanger network. In this paper, the pinch design method[4-8] is applied to obtain the optimal heat exchanger network.

As only phase change –latent heat transfer- occurs in the condensers and reboilers, the inlet and outlet temperatures of a stream can be considered as the same in the preliminary stage. So the temperature vs heat composite curves of hot streams and cold streams are both a cascade horizontal lines with different temperature level and different length, as shown in Fig.3. In such a situation it's easy to locate the pinch position.

The basic steps of determining the pinch position are:

Step 1. Stream temperatures are shifted either up (cold streams) or down (hot streams) by the chosen minimum temperature approach $T_{min.}$

Step 2. The shifted temperatures are then sorted in decreasing order. We denote the temperature sequence as $\{T_j\}$, and the corresponding enthalpy change sequence as $\{\triangle H_j\}$, $j=1,2,\ldots,n$. Where n is the number of streams for heat exchange. Note that for hot streams $\triangle H= Q_c$ and for cold streams $\triangle H= -Q_r$, meaning that the hot streams give out energy and the cold streams receive energy.

Step 3. The output energy Q_j is given by: $Q_j = -\sum_{m=1}^{j} \Delta H_m$, $j=1,2,\ldots,2n$. The point at which Q_j is the minimum represents a pinch point.

After the pinch position is founded, all the heat matches can be determined accordingly. For example, there are three matches in the case shown in Fig.3.

3.4. Formulation of optimization problem and solution approach

Based on the above analysis, the synthesis problem in this paper can be formulated as the following optimization problem

$$\text{Min } COST = \text{Min } C (p, \xi_{LK} , \xi_{HK} , r) \tag{1}$$

In this paper, the investment cost of column is estimated by the method suggested by Guthrie[9], the capital cost of condenser, reboiler, and exchanger is estimated based on the correlations and data provided by Douglas[10], while the operating cost is calculated based on the heat duty and utilities.

The cost function given by Eq. (1) is in general an implicit and nonlinear function. In this paper the simulated annealing algorithm is used to solve problem (1) with p, ξ_{LK} , ξ_{HK} and r as variables.

4. Illustrating Example

The example is a five-component mixtures separation problem. The feed flow is 100kmol.h^{-1}, The feed component and mole fractions are: A: n-pentane (0.1), B: n-hexane (0.1), C: n-heptane (0.2), D: n-octane (0.3), E: n-nonane (0.3), T_{min} is 10k, all desired products are their pure products and recovery in all columns is specified to be 98%.

Table 1 The available utilities

Utilities	Pressure, MPa	Temp., K	Cost, $.GJ^{-1}
(1) cooling water		305	0.0.67
(2) steam	0.170	389	0.418
(3) steam	0.408	418	0.574
(4) steam	1.122	458	0.774
(5) steam	2.824	503	1.03

The available utilities and their conditions are given in Table 1. The design

results for the given flowsheet of Fig.1a are shown in Table 2. There is one heat match between column 2 and 4. The heat integrated flowsheet is shown in Fig.1c.

Table 2 The design results for the flowsheet of Fig.1 of the example

Tasks	P, MPa	ξ_{LK}	ξ_{HK}	ξ_{MC}	R	Q_c , GJ^{-1}	Q_r , GJ^{-1}
ABC|CDE	0.177	0.9945	0.0050	0.2503	0.56	—	—
A|BC	0.177	0.98	0.02	—	4.12	1.266	—
B|C	0.177	0.98	0.02	—	1.62	0.710	—
C|DE	0.177	0.98	0.02	—	1.46	—	2.553
D|E	0.399	0.98	0.02	—	1.60	2.258	2.372

Cost=33692.82 \$.y^{-1}

Number of theoretical trays : N_t =[8, 73 ,9, 24]^T

Feed locations: F_t=[7, {11(ABC), 47(CDE), 9, 12}]^T

Product drawing locations: column 2: [24 (BC), 30 (C)]

Heat match: Q (4—2) =2.258 GJ^{-1}

5. Conclusions

The simultaneous heat integration and parameter optimization for a given complex distillation column flowsheet is studied. A general design procedure including converting a complex distillation column flowsheet into its thermodynamic equivalent simple column flowsheet, the shortcut design of the equivalent scheme, and design of the heat integration structure with pinch design method is developed. The example has shown that the design procedure can effectively give all the needed design parameters and heat integration structure.

References

1. N.A.Carlberg and A.W.Westerberg, Ind. Eng. chem. Res., 28(1989), 1369
2. C.Triantafyllou and R.Smith, Trans. IChemE., 70(1992), 118
3. B.G.Rong and A.Kraslawski, Computer Chem. Engng., 25(2001), 807
4. B.Linnhoff and J.R.Flower, AICHEJ., 24(1978), 633
5. B.Linnhoff and H.Dunford, Chem. Eng. Sci., 38(1983), 1175
6. M.A.Duran and I.E.Grossmann, American Institute of Chemical Engineers Journal, 32(1986),123
7. I.E.Grossmann and H.Yeomnas, Computer Chem. Engng.,22(1998),S157
8. I.E.Grossmann and H.Yeomnas, Computer Chem. Engng.,23(1999),1135
9. K.M.Guthrie, Chem. Engng., 24(1969), 114
10. J.M.Douglas, Conceptual Design of Chemical Process, McGraw-Hill, New York (1988)