Approximate design and cost evaluation of internally heat-integrated distillation columns (HIDiCs)

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Abstract-Commercial design programs do not provide a ready-to-use process simulation of tray-by-tray heat-integrated distillation columns, so the computation of the columns using the programs is difficult due to their convergence problem. An approximate procedure for the design of the internally heat-integrated distillation column (HIDiC) is proposed here, and its performance of the design and cost evaluation is demonstrated with two example processes. The approximate design procedure eliminates the artificial heat exchangers and in-tray streams required in the design with the commercial programs, and therefore no information of the exchangers and streams is necessary except the amount of the in-tray heat transfer rate. The economic evaluation indicates that a reduction of the total annual cost of 8.1% is possible with benzene-toluene process and that 59.3% is yielded with the propylene-propane process. The results also demonstrate that the HIDiC is especially efficient for the tight separation system.

Key words: Internally Heat-integrated Distillation, Energy-efficient Distillation, Approximate Design, Cost Evaluation

INTRODUCTION

Distillation is a separation process using large amounts of energy as the separation medium [1], and therefore its energy efficiency has been a major target in the study of its improvement. An obvious solution is heat integration between its condenser and reboiler, though they cannot be integrated directly for the heat recovery due to their unfavorable temperature difference. The reboiler temperature is higher than that of the condenser. A vapor compression or vacuum is applied to reverse the temperature difference and to make the heat recovery available. For improved heat recovery, the internally heat-integrated distillation column (HIDiC) [2-4] modifies the temperature distribution by increasing the pressure of the whole rectifying section of the distillation column instead of the condenser in the direct heat integration [5,6]. There are two drawbacks when the HIDiC is utilized instead of a conventional distillation system. The first is the installation of many heat transfer panels in trays. Especially, the rates of vapor flow are not uniform, and therefore the column diameter varies from the top to the bottom of column section. The construction of such a varying diameter column with many heat transfer panels is not simple. The other is the utilization of a compressor, which is expensive and difficult to operate and to maintain. This problem makes field engineers reluctant to apply HIDiC.

In the recent studies, heat integration with external heat exchangers has been proposed between trays in rectifying and stripping sections [7,8]. The problems of the compressor operation in the distillation column have been reported by Kataoka et al. [4]. The partial and internal heat integration without utilizing the compressor was applied to a ternary distillation column [9] and a quaternary system of two heat integrations [10], and some 17% and 28% of energy savings, respectively, were obtained. Though the HIDiC has not

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been commercially implemented, another energy-efficient distillation column, a divided wall column (DWC), is widely employed in many industrial processes [11-16]. But its application is restricted to ternary distillation systems, which limits its wide application. Another energy-efficient distillation column, a diabatic distillation column, has small heat exchangers in each tray for the reduction of the reboiler and condenser capacities of a conventional distillation column and the improvement of distillation column efficiency [17]. The reboiler and condenser are much smaller than those in the conventional distillation column. The heat transfers in the in-tray heat exchangers are at lower temperature than that of the reboiler and at higher temperature than that of the condenser, and therefore the exergy loss in the adiabatic distillation is much less than the conventional system [18,19]. However, the installation of small heat exchangers is difficult in practice.

In the studies of the internally heat-integrated distillation (HIDiC), no commercial software of distillation column design provides a ready-to-use heat-integrated column in the development of a process flow diagram. Instead, many external heat exchangers are used for the tray-by-tray heat transfers along with artificial streams from the trays, which require a large amount of stream information leading to the convergence problem in the process simulation of the HIDiC.

In this study an approximate design and simulation procedure with simple computation is proposed, and its performance is examined with two commonly used processes in the studies of the HIDiC design and cost evaluation. In the design of the HIDiC the installation of trays with internal heat integration is more difficult than the design of a conventional distillation column due to the heat transfer in trays. When commercial design software is used, the trays with the internal heat transfer are not readily provided. Many previous studies [20-22] utilized commercial software with the trays of external heat supplies, but the addition of heat supply and removal in each tray using an artificial modification is complicated when the tray numbers in the heat integration are large. The proposed design

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Fig. 1. A conceptual diagram of the internally heat-integrated distillation column (HIDiC).

procedure here calculates the tray composition from the material balance without using the commercial software, and therefore any modification in the trays is possible and the procedure is simple to apply for the HIDiC design.

DESIGN PROCEDURE

The conceptual structure of the internally heat-integrated distillation column is shown in Fig. 1. In a conventional distillation column the temperature of the rectifying section is lower than that of the stripping section, and therefore the tray-by-tray heat transfer demonstrated in the figure is not available. The vapor compression raises the temperature in the rectifying section, and the heat released from the rectifying section is recovered and supplied to the stripping section.

The material balance at a tray is given as

$$V_{i+1}y_{i+1} + L_{i-1}x_{i-1} - V_iy_i - L_ix_i + \delta_F qFx_F = 0$$
(1)

where the subscript j indicates tray number and counted from the top, and the feed is supplied only at the feed tray. Because the system is binary, no component indication is necessary. The feed quality q is determined from the flow rate of top product. The vapor and liquid flow rates are

$$\mathbf{V}_j = \mathbf{V}_{j+1} + \frac{\mathbf{Q}_j}{\lambda_j} \tag{2}$$

and

$$L_j = L_{j-1} - \frac{Q_j}{\lambda_j} \tag{3}$$

where Q_j is the amount of the transferred heat and λ_j is the heat of vaporization. The vapor-liquid equilibrium is formulated as

$$\mathbf{y}_{j} = \mathbf{K}_{j} \mathbf{x}_{j} \tag{4}$$

For the simplicity the relative volatility is used here to replace the equilibrium constant.

$$\mathbf{y}_j = \frac{\alpha}{1 + (\alpha - 1)\mathbf{x}_j} \mathbf{x}_j \tag{5}$$

The set of material balances is transformed to the matrix form, and an iterative procedure using a relaxation factor is applied to calculate the liquid composition.

$$\mathbf{A} \mathbf{X} = \mathbf{C} \tag{6}$$

where

Г

$$\mathbf{A} = \begin{bmatrix} -\mathbf{V}_{1}\mathbf{K}_{1} - \mathbf{L}_{1} & \mathbf{V}_{2}\mathbf{K}_{2} & \mathbf{0} & \mathbf{0} \\ \mathbf{L}_{1} & -\mathbf{V}_{2}\mathbf{K}_{2} - \mathbf{L}_{2} & \mathbf{V}_{3}\mathbf{K}_{3} & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \vdots \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \vdots & \vdots & \mathbf{0} \\ \mathbf{0} & \vdots & \mathbf{0} \\ \mathbf{L}_{NT-2} - \mathbf{V}_{NT-1}\mathbf{K}_{NT-1} - \mathbf{L}_{NT-1} & \mathbf{V}_{NT}\mathbf{K}_{NT} \\ \mathbf{0} & \mathbf{L}_{NT-1} & - \mathbf{V}_{NT}\mathbf{K}_{NT} - \mathbf{L}_{NT} \end{bmatrix}$$
(7)
$$\mathbf{C} = \begin{bmatrix} -\mathbf{L}_{0}\mathbf{x}_{D} \\ \mathbf{0} \\ \vdots \\ -\mathbf{F}_{L}\mathbf{x}_{F} - \mathbf{F}_{F}\mathbf{x}_{F} \\ \vdots \\ \mathbf{0} \\ - \mathbf{V}_{NT+1}\mathbf{K}_{NT+1}\mathbf{x}_{NT+1} \end{bmatrix}$$
(8)

The details of computation procedure are as follows:

1) Set total numbers of trays in the rectifying and stripping sections.

2) Set heat transfer area in tray and overall heat transfer coefficient.

3) Set the heat of vaporization and relative volatilities in the rectifying and stripping sections.

4) Set the flow rates of vapor and liquid feeds.

5) In case of ideal HIDiC, set liquid flow to the top tray and vapor flow to the bottom tray zero.

6) Set the relaxation factor between 0 and 1.

7) Set temperature difference in tray-by-tray pairing. This can be modified for rigorous computation using the VLE equation.

8) Calculate the rate of heat transfer at the trays in the heat transfer pairing.

9) Calculate the flow rates of liquid and vapor in trays.

10) Guess the initial liquid composition in trays using the linear distribution between the compositions of overhead and bottom products.

11) Formulate the matrix coefficients (7) and (8).

12) Calculate the new set of liquid compositions using matrix inversion.

13) Iterate the matrix computation using the new set of liquid compositions until the composition variation is less than a given limit.

14) If the specification of overhead and bottom products is not satisfied, adjust the temperature difference and go to step 7.

EXAMPLE PROCESSES

Two widely used processes in the HIDiC studies are employed in the evaluation of the proposed design procedures of this study. The benzene-toluene process [3] has been examined from the early studies in the field. The vapor-liquid equilibrium is close to ideal and their boiling points are relatively wide, resulting in easy separation. Two different relative volatilities are used here for the rectifying and stripping sections. All the trays of rectifying and stripping sections are involved in the heat transfer. The second process is a close boiling system of propylene-propane process [20-22]. Because the tight separation requires considerable energy demand in the conventional distillation system, many studies have been conducted to find an energy efficient process for the separation. Due to the feed condition the tray number of stripping section is less than the rectifying section, and the top of the rectifying section is paired in the heat transfer. The details of column structures and operating conditions are listed in Table 1. The column structure and operating conditions are summarized for either of the HIDiC and conventional distillation systems. In the HIDiC the rectifying section is operated at the elevated pressure to give sufficient temperature difference for the heat recovery, and the different relative volatilities are used for the rectifying and stripping sections. For a fair comparison, the HIDiC and conventional distillation systems are under similar conditions.

RESULTS AND DISCUSSION

The internally heat-integrated distillation column (HIDiC) has been introduced for the heat recovery from the rectifying section by raising its operating pressure to have the tray-by-tray heat transfer to the stripping section. Therefore, neither condenser nor reboiler is

S S S VNT+1

Lo

Fig. 2. A schematic diagram of the internally heat-integrated distillation column (HIDiC). The symbol S indicates the stripping section, and R does the rectifying section.

necessary in the ideal HIDiC. In practice, a small condenser and reboiler are installed for the startup of the distillation column. Fig. 2 shows the schematic diagram of the practical HIDiC. In case of benzene-toluene system the tray numbers of the rectifying and stripping sections are the same, and the tray-by-tray pairing is given from the top to the bottom of both sections. However, the propylene-propane system has different tray numbers, as given in Table 1. The utilization of the rectifying section needs to determine which portion of the section is paired with the stripping section, because the rectifying section has more trays than the stripping section. When the middle or bottom part of the rectifying section is used, the liquid flow increased due to the heat transfer does not affect the separation in the top portion of the rectifying section. In this case the distillation column efficiency is lower than the top portion pairing, and the same outcome has been published before [21,22]. In case of the benzene-toluene process the tray numbers in the conventional

Nama	Benzene-toluene		Propylene-propane		
Name -	HIDiC (rectifying/stripping) Conv. HIDiC (rectifying/stripping)		Conv.		
Structural					
Number of trays					
Total	64	50	270	270	
Rectifying/Stripping	32/32	25/25	150/120	150/120	
Heat transfer area in tray (m ²)	20		400		
Overall heat transfer coeff. (W/m^2K)	600		1000		
Operating					
Pressure (kg/cm ²)	2.55/1.0	1.0	14.6/11.2	11.2	
Relative volatility	2.06/2.35	2.35	1.13/1.15	1.15	
Feed (kmol/h)	300	300	2601.6	2601.6	
Feed quality	0.5	0.5	0.52	0.52	
Composition (mol frac.)					
Feed	0.5/0.5	0.5/0.5	0.52/0.48	0.52/0.48	
Product-overhead	0.995	0.995	0.995	0.995	

Table 1. Structural information, operating conditions and compositions in the proposed and conventional distillation systems. Tray numbers are counted from the top



Fig. 3. A search of the tray numbers having the minimum total annual cost calculated using the approximate design procedure in the conventional distillation columns.

distillation column are smaller than the HIDiC. The optimum number of trays for the conventional column was calculated as 50, but the HIDiC requires sufficient tray numbers for the heat transfer between the rectifying and stripping sections leading to more trays. The difference is explained in Nakaiwa et al. [3]. The design of the conventional distillation column used for the performance comparison utilized the same procedure with no in-tray heat transfer. The optimum number of trays is found from the comparison of the total annual cost as plotted in Fig. 3. The tray numbers of 50 and 270 for the benzene-toluene and propylene-propane systems, respectively, are determined from the figure. When the number of trays is increased, the cost of column construction increases while the utility cost is reduced. Therefore, the total annual cost is considered to determine the optimum number of trays. In both example processes, as the tray numbers are elevated, the total annual cost decreases steadily until the minimum. After the minimum the cost increases as the number is raised to increase the capital cost more than the utility cost. In the propylene-propane process the number of trays is sufficient enough for the heat transfer, and therefore both the HIDiC and conventional distillation systems use the same number of trays. The heat transfer area and the overall heat transfer coefficient were determined from the guidelines of Olujic et al. [20].

As shown in Fig. 2 the cross sectional area of the rectifying section is increased as moved to the bottom due to the added liquid flow from the heat transfer to the stripping section, while the cross sectional area of the stripping section is reduced as the tray goes down. Therefore, the whole diameter of the combined column can be set near to the constant diameter. The required heat transfer area in trays is not sufficient with only the wall area between the two sections. Installing the additional heat transfer panels was proposed and the available area was indicated in [23]. The necessary area in this study can be obtained from the additional panels. The installation of the panels is available in the stripping section at the top of the distillation column, and that is possible in the rectifying section at the bottom. In the middle both the sections can be used for the panel installation. The heating panels in a concentric heat-integrated column for the heat transfer between the rectifying and stripping



Fig. 4. A cross-sectional diagram of the tray installed with heating panels in a concentric heat-integrated column.

sections are demonstrated in Fig. 4.

The computation of vapor-liquid equilibrium is approximated with using the relative volatility in this study of the approximate design, but the equilibrium of the systems used here is close to the ideal and the approximation does not leave a large computational error. Fig. 5 demonstrates the difference between the rigorous and approximate computations, which does not show noticeable discrepancy. The circles are from the experimental data and the rigorous VLE computation, and the curve is calculated from the relative volatility. Because most of close boiling point systems are composed of chemical compounds having similar chemical structure, the approximate VLE computation using the relative volatility is suitable for the system simulation.

The results of economic evaluation are listed in Table 2. The investment and operating costs are evaluated using the procedures [3,20,24,25], and a recent M&S index is used. The cost of utilities is very critical to determine the economic comparison of the total annual cost for the HIDiC and conventional columns. The data used



Fig. 5. A comparison of vapor-liquid equilibrium computed from the rigorous (circles) and approximate (curve) equations. Top is the system of benzene-toluene, and bottom is of propylene-propane.

Table 2.]	Economic	evaluation	of the	proposed	and cor	iventional
	distillation	i systems. U	J nits a	re in milli	on U.S.	dollars

Nama	Benzene	e-toluene	Propylene-propane		
Indiffe	HIDiC	Conv.	HIDiC	Conv.	
Investment					
Column	0.907	0.569	23.24	17.35	
Tray	0.088	0.0505	7.734	5.496	
Heat exchanger		0.415		3.493	
Compressor	1.627		11.48		
Utilities					
Steam		0.477		15.09	
Cooling water		0.0348		0.763	
Electricity	0.303		3.286		
Total annual cost	0.566	0.616	7.531	18.49	

in Nakaiwa et al. [3] was adopted in this study. The investment cost is counted with the 10 year payback. The investment cost of the compressor takes a large portion in both processes, and the steam and electricity costs are the main in the utility cost. While the cost comparison in the benzene-toluene process gives a mild improvement of 8.1% in the HIDiC, that in the propylene-propane process does a large improvement of 59.3%. Because the process is a close boiling point process requiring a large amount of tray numbers and steam consumption, the steam cost has a significant role in the cost comparison. Therefore the HIDiC is more useful in the tight separation processes. In the ideal HIDiC none of reflux flow or vapor boilup is necessary, because the liquid flow is obtained from the heat transfer at the top tray and throughout the rectifying section and the vapor flow is given at the bottom tray and throughout the stripping section. Therefore the condenser and reboiler are not considered in the cost evaluation of the HIDiC. The design results of two example processes are compared with the previous studies [3,20] in Table 3. When the same specification of products is yielded, the column designs are listed with the cost evaluation. The total numbers of trays are about 20% different in both processes due to the difference of payback time. Though the investment and utility costs are close in the benzene-toluene process, they are different in the propylene-propane process. The difference is from the value of the Marshall and Swift index and the tray spacing. The values are given in the cost evaluation equations listed in the appendix.

CONCLUSIONS

An approximate procedure for the design of the internally heatintegrated distillation column (HIDiC) is proposed here, and the performance of the column design and cost evaluation is examined with two example processes. Though many commercial programs are used in the design of distillation columns, no ready-use program for the heat-integrated column is available. The proposed approximate procedure eliminates the artificial heat exchangers and in-tray streams required in the design with the commercial programs. The proposed procedure shows how simple the design of the HIDiC is, and the economic evaluation indicates that a reduction of the total annual cost of 8.1% is possible with the benzenetoluene process, and that 59.3% is yielded with the propylene-propane process. This result demonstrates that the HIDiC is especially good for the tight separation system.

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Table 3. Comparison of the design results and cost e	valuation of this study with prev	vious studies. Tray nu	ambers are counted from the
top. Cost units are in million U.S. dollars			

	Benzene	toluene	Propylene-propane	
Name	This study	Ref. 3	This study	Ref. 20
	(rectifying/stripping)		(rectifying/stripping)	
Structural				
Number of trays				
Total	64	80	270	231
Rectifying/Stripping	32/32	40/40	150/120	170/61
Overall heat transfer coeff. (W/m ² K)	600	600	1000	1000
Operating				
Pressure (kg/cm ²)	2.55/1.0	2.55/1.0	14.6/11.2	14.6/11.2
Feed (kmol/h)	300	300	2601.6	2601.6
Feed quality	0.5	0.5	0.52	0.52
Composition (mol frac.)				
Feed	0.5/0.5	0.5/0.5	0.52/0.48	0.52/0.48
Product-overhead	0.995	0.995	0.995	0.996
Costs				
Investment	2.62	2.56	42.45	20.08
Utilities	0.30	0.30	3.29	5.03

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NOMENCLATURE

- A : coefficient matrix in Eq. (7) [-]
- B : bottom product [-]
- C : coefficient matrix in Eq. (8) [-]
- D : overhead product [-]
- F : feed flow rate $[\text{kmol } h^{-1}]$
- K : equilibrium constant [-]
- L : liquid flow rate [kmol h^{-1}]
- Q : heat transfer rate $[kJ h^{-1}]$
- q : vapor portion in feed [-]
- R : rectifying section [-]
- S : stripping section [-]
- V : vapor flow rate [kmol h^{-1}]
- **X** : liquid composition matrix in Eq. (6) [-]
- x : liquid composition [-]
- y : vapor composition [-]

Subscript

- 0 : flow to top tray
- D : overhead product
- F : feed tray
- j : tray number
- L : liquid
- NT : total number of trays
- V : vapor

Greek Letters

- α : relative volatility [-]
- δ : feed tray index [-]
- λ : heat of vaporization [kJ kmol⁻¹]

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APPENDIX

The evaluation of column cost is given as

$$C_{col} = \left(\frac{M \& S}{280}\right) C_{j} D_{c}^{1.066} H_{c}^{0.802} C_{p}$$
(A1)

where the M&S is the Marshall and Swift index and the value of 3^{rd} quarter of 2010 of 1473.3 is used here. The pressure related cost coefficient C_f is given in Olujic et al. [20]. The column diameter is found from

$$D_c = 0.1838 \times 0.3048 \sqrt{V}$$
 (A2)

where V is the rate of vapor in lb-mol/h. The height of column is calculated from two inch spacing and the total number of trays. The penalty coefficient C_p of 1.2 was used for the HIDiC. The cost of trays is

$$C_{tray} = \left(\frac{M \& S}{280}\right) 97.243 D_{C}^{1.55} H_{C} F_{c} C_{p}$$
(A3)

where the fabrication coefficient F_c is given in Olujic et al. [20]. The condenser cost is

$$C_{cond} = \left(\frac{M \& S}{280}\right) 1609.13 A_{C}^{0.65}$$
(A4)

where A_c is the heat transfer area of the condenser. Similarly, the reboiler cost is

$$C_{red} = \left(\frac{M \& S}{280}\right) 1775.26 A_R^{0.65}$$
(A5)

The cost of compressor is calculated from

$$C_{comp} = \left(\frac{M \& S}{280}\right) 2047.24 b_{P}^{0.82}$$
(A6)

where b_p is found from the previous reference. The cost of electricity is \$0.0843 per kWh, and the steam and cooling costs are \$13 per ton and \$0.03 per ton, respectively.