

Approximate Design of Fully Thermally Coupled Distillation Columns

Young Han Kim[†], Masaru Nakaiwa* and Kyu Suk Hwang**

Dept. of Chem. Eng., Dong-A University, Busan 604-714, Korea

*Energy-Efficient Chemical Systems Group,

National Institute of Advanced Industrial Science and Technology, Tsukuba 305-8565, Japan

**Dept. of Chemical Engineering, Pusan National University, Busan 609-735, Korea

(Received 15 November 2001 • accepted 16 January 2002)

Abstract—An approximate design procedure for fully thermally coupled distillation columns (FTCDCs) is proposed and applied to example ternary systems. The procedure gives a fast solution of structural and operation design for a preliminary study of the FTCDC. The structural information resolves the design difficulty, caused from the interlinking streams of the column, which is encountered when a conventional design procedure is implemented. The design outcome explains that how the thermodynamic efficiency of the FTCDC is higher than that of a conventional two-column system and how the system of a separate prefractionator is different from a dividing wall structure. From the design result of three example systems with three different feed compositions, the useful performance of the proposed scheme is proved. In addition, the structural design of the FTCDC gives better understanding of the system and leads to high efficiency design of the column.

Key words: Process Design, Distillation Column Design, Thermally Coupled Distillation, Approximate Design, Energy Efficient Distillation

INTRODUCTION

Though a fully thermally coupled distillation column (FTCDC), the Petlyuk column [Petlyuk et al., 1965], was introduced almost half a century ago, it was not commercially implemented until recently owing to the difficulty of its design and operation [Abdul Mutalib et al., 1998a]. However, several industrial applications have been reported lately [Woff and Skogestad, 1995; Midori and Nakahashi, 1999; Lestak et al., 1999], and its wide utilization is expected in a variety of separation processes.

For the separation of ternary mixtures, the FTCDC requires less energy compared with a conventional distillation system utilizing two distillation columns in various feed compositions [Fidkowski and Krolokowski, 1986]. The energy saving in the FTCDC is mainly from the elimination of the remixing of intermediate component in the first column and the reduction of mixing effect in the feed stage of a conventional distillation system [Triantafyllou and Smith, 1992]. Usually, heat integration in a conventional distillation system is conducted by arranging heat exchangers to recover wasted energy as much as possible. The thermodynamic efficiency of the distillation system is examined from energy calculation [Yoo et al., 1988]. Also, a new simulation procedure employing a rate-based model was proposed by Lee et al. [1997].

In the early studies, the minimum reflux flow rate of the FTCDC was investigated by many researchers [Glinos and Malone, 1985b; Fidkowski and Krolokowski, 1986; Carlberg and Westerberg, 1989] in order to analyze column characteristics and to find an optimum operating condition. While the former two studies dealt with a ternary mixture, the last explained the minimum reflux flow of gen-

eral cases. All of them are based on Underwood's original works [Underwood, 1948, 1949].

In conventional distillation design, liquid flow rate and the number of trays are inversely proportional and the relation is continuous unless either of the values is less than its minimum. But this is not applied to the FTCDC. The result of Wolff and Skogestad [1995] shows that no separation is available with some split of liquid flow between a main column and a prefractionator. The split for a given separation has upper and lower limits, and there is a curve to show the relation between the split and vapor boilup. However, the curve is disconnected in the middle, where even infinite amount of vapor boilup does not give a desired separation. Therefore, it is difficult to apply a conventional design to the FTCDC.

Although the minimum reflux flow rate has been widely investigated, the structural design information, such as the number of trays in a prefractionator and a main column and stages of feed, side product and interlinking between the two columns, has not been studied. For the structural design, a short-cut design of the FTCDC was proposed by Triantafyllou and Smith [1992]. By separating the main column into two, the short-cut design equations for multi-component distillation can be separately applied, and the design procedure of the three-column model is formulated. In the study, the minimization of total cost including capital and energy costs was conducted to find an optimum design of the FTCDC. However, linking the separated two columns requires an adjustment for the match of vapor and liquid flow rates of both columns to result in an iterative recalculation of stage numbers of both columns. Also, the short-cut design leaves an accuracy problem as shown from the large difference between the design and the rigorous design as shown in the study.

Commercial process design tools can also be utilized in the design of the FTCDC, but lack of the structural design information needs

[†]To whom correspondence should be addressed.

E-mail: yhkim@mail.donga.ac.kr

numerous iterative computations until required product specification is yielded. Moreover, inadequate column structure often gives a convergence problem.

The short-cut method [Seader and Henley, 1998] for a multi-component distillation column is also not applicable to the design of the FTCDC owing to the unknown compositions of interlinking streams. On behalf of the short-cut method, an approximate design method utilizing an ideal equilibrium and a set of material balances is proposed here.

In this study, an approximate design procedure to find the structural column information, such as the number of trays of a prefractionator and a main column, feed and side product stages and interlinking location between the prefractionator and main column of the FTCDC, is proposed and examined for the design performance by implementing it to example designs. The operational variables are yielded from the solution of material balances.

The structural information is also analyzed to examine thermodynamic efficiency of the distillation system. The investment and operational cost of the FTCDC is compared with a conventional two-column system. While a rigorous design requires long computation time, this approximate design needs a fraction of the time and many different arrangements can easily be evaluated in the stage of preliminary process design until a final decision is made. The proposed design procedure can satisfy such a demand.

DEGREES OF FREEDOM

The schematic diagram of an FTCDC, also known as the Petlyuk column, is given in Fig. 1. The column has a single set of reboiler and condenser unlike a conventional two-column system for the separation of a ternary mixture.

The analysis of the degrees of freedom of the FTCDC gives important information for structural design and the selection of manipulated and controlled variables necessary for column operation. Few previous studies [Wolff and Skogestad, 1995; Cerda and Westerberg, 1981] analyzed the characteristics of the FTCDC and found some possible operational strategies.

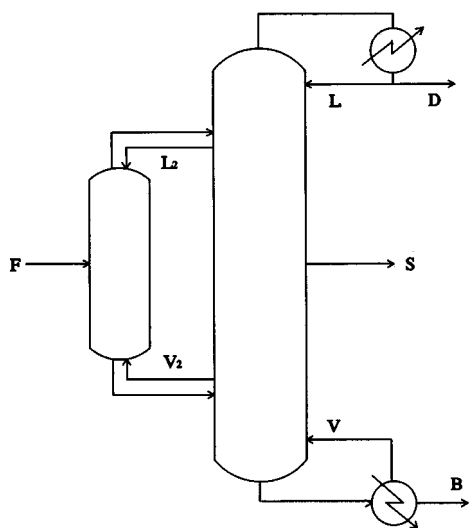


Fig. 1. Schematic diagram of a fully thermally coupled distillation column.

Table 1. Degrees of freedom analysis

Unknowns	Number
Numbers in trays	6 (NT, NT ₂ , NF, NP, NR, NS)
Flow rates in operation	2 (VC, RP)
Liquid composition	(NT+NT ₂ +2)NC
Vapor composition	(NT+NT ₂ +1)NC
Vapor boil-up rate	1
Reflux flow rate	1
Total	(2NT+2NT ₂ +3)NC+10
Equations	Number
Component material balance	(NT+NT ₂ +2)NC
Equilibrium relation	(NT+NT ₂ +1)NC
Total	(2NT+2NT ₂ +3)NC
Degrees of freedom	10

In Table 1, all the variables appearing in the design and operation are listed, and the numbers of balance equations and equilibrium relations are counted. Liquid and vapor compositions are given for all the trays of a prefractionator and a main column. While equilibrium is obtained in a reboiler, no equilibrium is formed in a total condenser. The additional number of two in stage number denotes a reboiler and a total condenser, and the one in equilibrium indicates the equilibrium of the condenser. As a result, 10 degrees of freedom are found from the analysis.

The ten are divided into two groups: structural design related variables and operation related variables. The six structural variables are the numbers of stages of a prefractionator and a main column, feed and side product locations and two interlinking stages between the prefractionator and the main column. The four operational variables are reflux flow rate, vapor boil-up rate, liquid split ratio from the main column to the top of the prefractionator and vapor split ratio from the main column to the bottom of the prefractionator. While all of lightest component in feed goes to a main column through the top of a prefractionator, a split of middle component in feed is transferred along the stream. Namely, the vapor flow from the top of the prefractionator is the combined amount of the liquid flow from the main column to the prefractionator and the flow of the lightest and the split of middle component in feed. In steady state design, the vapor split ratio is readily found when the split of the middle component is given. The computational detail of design is given below and summarized in Fig. 2.

STRUCTURAL DESIGN

In the design of a conventional distillation column, the number of trays is calculated by using various design equations by setting the reflux flow rate at between 1.2 and 2.0 times the minimum reflux flow rate [McCabe and Smith, 1976]. Otherwise, an optimization for the minimization of total annual expense including capital cost and energy expense is conducted to find the optimum reflux flow rate. Using the optimum reflux flow rate, the number of trays of the distillation column is readily obtained, but the procedure is not applicable to the design of an FTCDC owing to unknown information of the location of interlinking stages and the composition of interlinking streams.

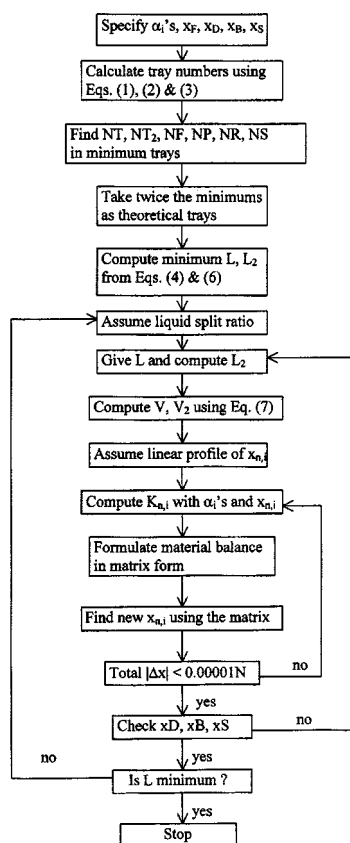


Fig. 2. Computation sequence of the proposed design.

Instead, the minimum numbers of trays of a prefractionator and a main column are computed first by using an approximate design procedure here. The stage locations of feed, side product and interlinking between a prefractionator and a main column are also obtained from the procedure. Then, all the tray-related numbers are proportionally increased for a practical distillation column. There are some advantages to this procedure. Because the practical design is derived from the minimum tray design based on ideal tray efficiency, it is ensured that the design is the most efficient thermodynamically. This practice has been applied to the design of extended FTCDCs [Kim, 2001]. Although many commercial design programs are available for multi-component distillation systems, none of them provides the structural information, and numerous iterative computations have to be conducted in the search of an optimum structure. The proposed design procedure helps to eliminate the computational load.

From the residue curves of simple distillation of a ternary mixture shown in Fig. 3, it is noticed that the ternary distillation lines vary widely according to operational variables, such as liquid and vapor flow rates. Though the curves represent the composition profile of a packed column operated in total reflux and distillation lines follow that of a tray column, both curves have a similar pattern. For the simplicity of explanation, the residue curves are used here. The increase of liquid flow moves the residue curve close to the vertex, representing the intermediate component, of a triangular ternary composition diagram. It means that higher composition of intermediate component in side product is available with the increased liquid flow while light and heavy products have little change of com-

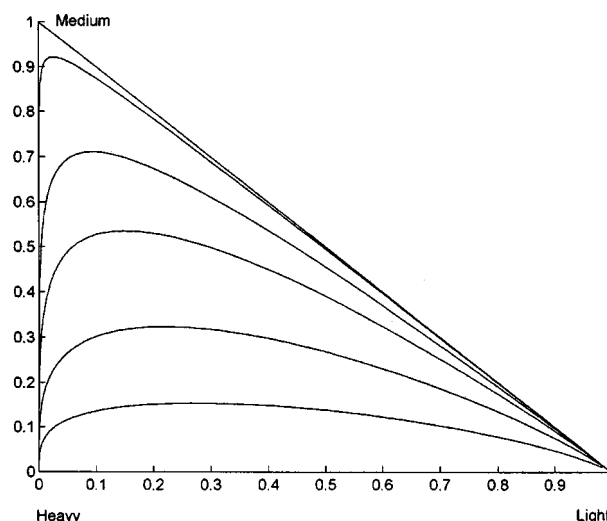


Fig. 3. Residue curves of a ternary distillation system.

position. In other words, the composition of side product determines the path of the distillation line for a main column. If a feed composition is not far from the feed stage composition, it also decides the path of a prefractionator. Unless the compositions of intermediate component in feed and side product are close, the distillation lines of a prefractionator and a main column are distant owing to the difference of the compositions. If the composition of intermediate component in feed is much smaller than that in side product, the distillation line of a prefractionator is far from the vertex of a triangular liquid composition diagram while the distillation line of a main column is close to the vertex. Because the distillation lines of the main column and prefractionator of an FTCDC have similar pattern to the residue curves, the FTCDC has high thermodynamic efficiency. A distillation line from one of the residue curves means ideal tray efficiency with no irreversible feed tray mixing. A detailed explanation of this subject is in Kim [2002].

This is overlooked in many studies [Triantafyllou and Smith, 1992; Chavez et al., 1986; Annakou and Mizssey, 1996; Abdul Mutalib et al., 1998b; Dünnebier and Pantelides, 1999], and the dividing wall structure is adopted to take the advantage of simple construction. In the dividing wall structure, tray numbers of a prefractionator and the middle section of a main column are adjusted to be equal in spite of the difference of distillation lines. Consequently, mismatch-caused by the intentional adjustment-of the compositions of feed and feed stage is generated to lower the thermodynamic efficiency of the system. In the rigorous design of Triantafyllou and Smith [1992], it is found that the number of prefractionator stages is less than that of the mid-section of a main column although their short-cut design gives an equal number. This outcome supports the explanation of feed stage composition mismatch.

In the design of a main column, the Fenske multi-component design equation is applied.

$$N_{min} = \frac{\log \{ [x_{i,N+1}/x_{i,1}] [x_{j,1}/(x_{j,N+1})] \}}{\log \alpha_{i,j}} \quad (1)$$

In order to follow the residue curve including side product composition, the computation of tray number is conducted separately in two sections: upper and lower sections from the tray of side prod-

uct. For the upper section of the column, the lightest and intermediate components are used in Eq. (1), and the intermediate and heaviest components are for the lower section.

The design of a prefractionator cannot follow the above procedure, because the end compositions are unknown. Therefore, a stage-to-stage computation is proposed here. Assuming that the feed stage has equal liquid composition to the composition of a saturated liquid feed and the tray efficiency is ideal, one can calculate the liquid composition of the stages above the feed tray from Eq. (2).

$$x_{n+1,i} = \alpha_{i,i} x_{n,i} / \sum_j \alpha_{j,i} x_{n,j} \quad (2)$$

where the subscript n denotes the n^{th} tray counted from the bottom and α is relative volatility. This computation continues until the composition of the heaviest component is less than that in side product. If the composition is higher than that of side product, the specification of side product cannot be met. The composition increases along down the trays from the upper interlinking tray, and therefore it has to be less than the specification at the interlinking tray.

Similarly, the liquid composition of the stages below the feed tray is calculated from

$$x_{n-1,i} = x_{n,i} / \left[\alpha_{i,i} \sum_j (x_{n,j} / \alpha_{j,i}) \right] \quad (3)$$

In this case, the computation proceeds until the composition of the lightest component is below that of side product as in the design of the upper section. Now the tray numbers of upper and lower sections give the total number of trays of the prefractionator. In addition, the selection of the tray having the closest composition with the ends of the prefractionator gives the location of interlinking trays in the main column. Because the tray numbers of upper and lower sections are given, the locations of feed and side product trays are readily determined. Note that the feed location has strong impact on the product composition owing to mixing at the tray.

The number of trays in a practical distillation column is taken as twice the minimum number estimated from the above. The factor of two in the computation of a practical column from the minimum tray column is common practice for the optimum number of trays. [Glinos and Malone, 1985a; Seader and Henley, 1998] Other tray-related numbers are proportionally increased to maintain the structure of the minimum tray design having ideal tray efficiency. Because the structure of the present design keeps that of the minimum design, the thermodynamic efficiency of the system is the highest among various available structures for an FTCDC.

OPERATIONAL VARIABLES

There are four operational variables, reflux flow rate, vapor boil-up rate, liquid and vapor split ratios between a main column and a prefractionator. Among them, two are eliminated in steady state calculation with the equimolal overflow assumption. Namely, the vapor boil-up rate is found from the reflux flow rate and overhead product rate. The vapor split ratio is also derived from the liquid split ratio and the flow rate of side product as explained below.

In the calculation of minimum liquid flow rate [Fidkowski and Krolkowski, 1986], the minimum flow of a main column is estimated as

$$L^{\min} = \max \left\{ \frac{A\phi_1}{\alpha_A - \phi_1}, \frac{A\phi_2}{\alpha_A - \phi_2} + \frac{\alpha_B B}{\alpha_B - \phi_2} \right\} \quad (4)$$

where ϕ 's are the solutions of the following equation [Underwood, 1948] for a saturated liquid feed.

$$\frac{\alpha_A A}{\alpha_A - \phi} + \frac{\alpha_B B}{\alpha_B - \phi} + \frac{\alpha_C C}{\alpha_C - \phi} = 0 \quad (5)$$

This is the total amount of liquid flow rate of a main column and a prefractionator. The minimum liquid flow rate [Fidkowski and Krolkowski, 1986] of the prefractionator is

$$L_2^{\min} = \frac{\alpha_C F}{\alpha_A - \alpha_C} \quad (6)$$

The middle component in feed is separately transported to a main column through either top or bottom of a prefractionator. The optimum split ratio of the middle component from the top of the prefractionator for the minimum liquid flow is given as

$$\beta = \frac{\alpha_B - \alpha_C}{\alpha_A - \alpha_C} \quad (7)$$

If the liquid split ratio is yielded with Eqs. (4) and (6), the vapor split ratio is easily obtained by using Eq. (7) and the flow rate of side product.

Among the four operational variables, tear variables are two liquid flow rates. Since the equimolal overflow assumption is utilized, the vapor flow rate of the main column is readily found when the liquid flow rate of the column is given. Also, the optimum split of the intermediate component is found from Eq. (7) and all of the lightest component goes to a main column from the top of a prefractionator. These and the liquid flow rate of the prefractionator give the vapor flow of the prefractionator.

The liquid flow rate of the main column is determined by checking the composition of products. If the composition does not meet the given specification, the flow rate is adjusted until the specification is satisfied. The liquid flow of the prefractionator is initially found from the liquid flow rate of the main column and the ratio of minimum liquid flows computed from Eqs. (4) and (6). Since the minimum flows are conservative [King, 1980], the ratio has to be examined by inspecting if the liquid flow rate of the main column is the minimum. The detailed procedure explained here is given in Fig. 2.

A procedure [Wang and Henke, 1966] for the composition calculation of a multi-component distillation is modified for an FTCDC. The vapor composition is replaced with a liquid composition and an equilibrium relation given with a constant relative volatility.

$$y_{n,i} = \alpha_{i,i} x_{n,i} / \sum_j \alpha_{j,i} x_{n,j} \quad (8)$$

The material balance is written in a matrix form, and an iterative computation is employed because the initial liquid composition is unknown to be assumed. In order to improve the convergence of the iterative composition calculation, a relaxation is added to the renewal of liquid composition. The factor of 0.3 is implemented in this study since fast convergence is obtained with the value. The convergence limit is set to 1.0E-5 times number of components times number of trays. When the sum of the differences in absolute value

between the compositions of new and one iteration ahead is less than the limit, the iterative computation stops. The calculated compositions of overhead, bottom and side products are compared with the specified product compositions. For instance, when the composition of the lightest component in overhead product is over 0.95, the given liquid flow rates are accepted and the computation goes forward. Kim [2000] provides more details of the simulation.

EXAMPLE SYSTEMS

Though an arbitrary set of relative volatility can be used as an example design, three actual systems are selected for practical demonstration. A generalized study with wide range of relative volatility may give useful information for later investigation. But since it takes too much computational work only three systems with three different feed compositions are examined here.

The examples are ternary systems of methanol-ethanol-water (I), cyclohexane-n-heptane-toluene (II) and s-butanol-i-butanol-n-butanol (III). The first is an aqueous alcohol solution, the second is a mixture of aliphatic and aromatic hydrocarbons and the last example is an alcohol isomer mixture. Though the combination of relative volatility of the systems is not widely different, the systems are selected from various species. Three different feed materials consist of an equimolar mixture (F1) and two mixtures of the composition of 0.75-0.125-0.125 (F2) and 0.125-0.75-0.125 (F3) in mole fraction. In the selection of feed composition, it is presumed that the impact of high concentration of the lightest component in feed on column design is similar to that of the heaviest component, and the composition combination of 0.125-0.125-0.75 is eliminated. The specification of overhead product is set to 0.95 of the lightest component in mole fraction, bottom product is 0.95 of the heaviest component and side product is 0.90 of the intermediate component. The relative volatility is computed from the experimental data [Gmehling et al., 1980] and the values are 2.76, 1.81 and 1.0 for the system I, 2.34, 1.49 and 1.0 for the system II and 1.93, 1.46 and 1.0 for system III. A feed of 300 moles per hour is provided for all systems.

RESULTS AND DISCUSSION

Owing to interlinking streams, a usual design procedure for multi-component distillation columns is not applicable to the design of an FTCDC. Therefore, an alternative design procedure utilizing the minimum tray structure is proposed here. The fact that the structure is based on ideal tray efficiency and there is no mixing at feed tray ensures high thermodynamic efficiency of the proposed design.

When an equimolar liquid feed is introduced, the liquid composition for the minimum number of trays for the system I with feed F1 is demonstrated in Fig. 4. The + symbols indicate the liquid composition of a prefractionator of which the computation begins with feed composition. Similarly, the o symbols are of a main column and the estimation is initiated from the composition of side product. The numbers of trays of the prefractionator and the main column are found from the figure along with the feed stage and the location of the side product. Also, the interlinking stages of the main column and the prefractionator are found by matching the composition of both ends of the prefractionator to close location in the main column.

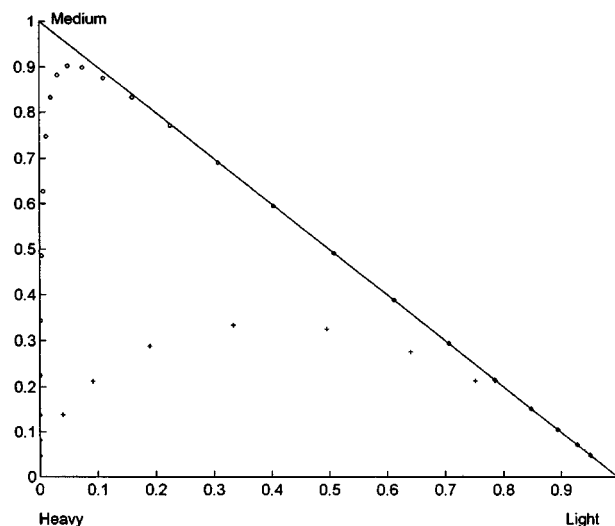


Fig. 4. Liquid composition in a fully thermally coupled distillation system at the minimum number of trays.

For the comparison of the fully thermally coupled distillation system with a conventional distillation of an example system, the system I with feed F1, a direct sequence two-column system is selected from the design suggestion of Glins and Malone [1988]. Note that ethanol and water make an azeotropic mixture and the direct sequence is inappropriate for the real process, but the formulation of the azeotropic mixture is ignored since an ideal equilibrium is assumed in this study.

The minimum number of trays is found by using Eq. (1) and the tray composition is shown in Fig. 5. The composition of the first column is depicted with + symbols, and the o symbols are of the second column. The actual number of trays is twice the minimum as employed in the design of the FTCDC. Since the composition of bottom product of the first column is equal to that of feed stream of the second column in the direct sequence conventional distillation, the composition calculation of the first column begins with the feed composition of the second column. In order to have the

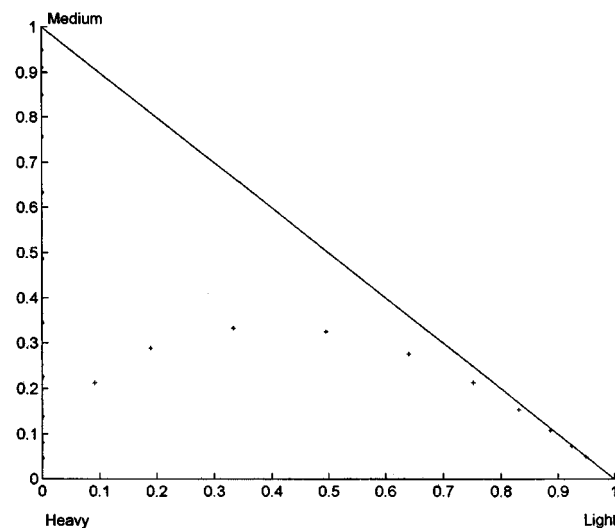


Fig. 5. Liquid composition in a conventional direct sequence two-column system at the minimum number of trays.

specified products of overhead and bottom from the second column of the conventional direct sequence ternary separation, the feed composition to the second column has to be fixed, and it is also of the bottom product of the first column. In the design of the first column, however, its feed composition and a possible feed stage composition have a large difference. Therefore, the feed composition is not considered in the design procedure. The large discrepancy between the feed composition and the feed stage composition of the first column induces significant mixing at the tray, which reduces the thermodynamic efficiency of the system.

As explained above, twice the minimum tray number is taken as the tray number of a practical distillation system, and steady state simulation is conducted to find the liquid composition profile of the conventional distillation system. The profile for example system I with feed F1 is exhibited in Fig. 6, where the symbols are the same as in Fig. 4. Also, the design result for three example systems is summarized in Table 2, in which the structural and operational information is listed. There are a couple of points to explain the design outcome. The stage number of a main column is not affected from the feed composition because its distillation curve does not include the feed composition. On the other hand, the stage number of a prefractionator varies with different feed compositions. This argument applies to the tray locations of feed and side product. High

composition of the lightest component in feed requires low liquid flow rate in the table. The component of the largest amount leaves the top of the main column, and therefore a small portion of the liquid returns to the column.

Meanwhile, the composition computation for the second column of a conventional two-column system starts from feed composition, and Eqs. (2) and (3) are implemented for rectifying and stripping sections, respectively. Though the second column contains a small amount of impurity, the lightest component, the feed composition of the second column is assumed to be binary for computational purposes. When the third component is included in the computation, the design for the rectifying section of the column does not give a specified overhead product having high composition of intermediate component. Therefore, a binary assumption has to be implemented. The composition of the third component is so small that the assumption does not lead to large design error. The conventional distillation system can be designed with a common procedure, but the proposed design procedure of this study is implemented for a fair comparison between the conventional distillation column and the FTCDC. Twice the minimum tray number is taken as a practical tray number. The number of trays in the first column is found to be 35 and the second is 21, and feed locations are 10th tray from the bottom for both columns. The liquid composition profile of the actual system is shown in Fig. 7.

When the reflux flow rate of the FTCDC is compared with the minimum reflux flow rate, it is found to be 1.33 times the minimum which is within the range of common practice. Therefore, the tray number taken in this design, twice the minimum number of trays, is quite reasonable. As indicated in Glinos and Malone [1985a] and Seader and Henley [1998], the factor of two is from industrial practice and is a widely accepted guideline. However, the liquid flow rate of a prefractionator is less than the predicted amount from the minimum flow given by Eq. (6). As King [1980] noted that the equation computing the minimum flow for a multi-component system is conservative, the estimated minimum flow of the case of this study may be larger than true minimum. Therefore, the estimated liquid split found from the equation for the minimum flow has to be checked.

Unlike other designs [Triantafyllou and Smith, 1992; Chavez et al., 1986; Annakou and Mizssey, 1996; Abdul Mutalib et al., 1998b; Dünnebier and Pantelides, 1999], the number of trays of the prefractionator (14) is different from the number of trays of the mid-section of the main column (33) in the example system I. This prevents the column from being constructed in a dividing wall structure, which has equal tray numbers for the prefractionator and the mid-section. The equilibrium relation of a ternary mixture for the system having quite different composition between feed and side product does not guarantee an equal number of stages. Therefore, a separate prefractionator is inevitable. Otherwise, the thermodynamic efficiency is reduced by intentional matching of the tray numbers to introduce remixing of intermediate component in the prefractionator as in the first column of a conventional two-column system. When 10 trays of a main column are moved to a prefractionator to make an equal number in the prefractionator and the mid-section for dividing wall structure, a steady state simulation indicates that 0.5% more reflux flow is required at the same liquid split. However, at the optimal split of the dividing wall column 8.4% less

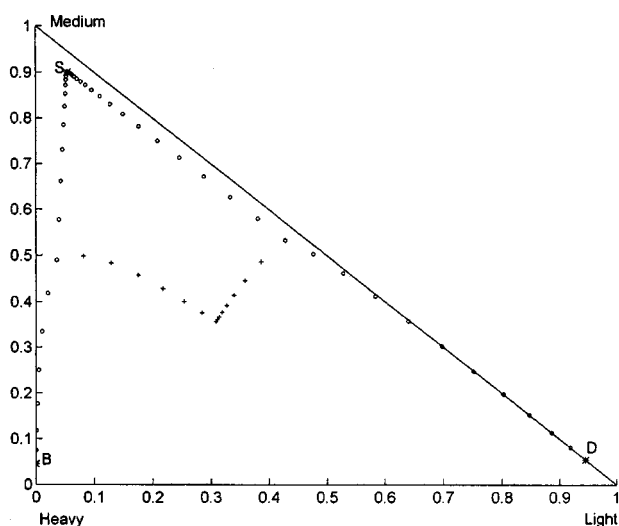


Fig. 6. Liquid composition in a fully thermally coupled distillation system at an actual number of trays.

Table 2. Design result of example systems

System	Feed	NT	NT ₂	NS	NR	NF	NP	L	V	L ₂
I	F1	49	14	7	39	7	19	557	656	133
	F2	49	16	3	43	11	19	379	614	91
	F3	49	20	11	39	3	13	523	550	88
II	F1	57	22	7	49	11	29	739	840	142
	F2	57	18	5	51	13	29	397	633	209
	F3	57	18	21	47	3	21	778	811	130
III	F1	74	20	10	58	9	30	951	1050	273
	F2	74	22	6	68	15	30	721	956	207
	F3	74	20	22	54	3	24	795	821	190

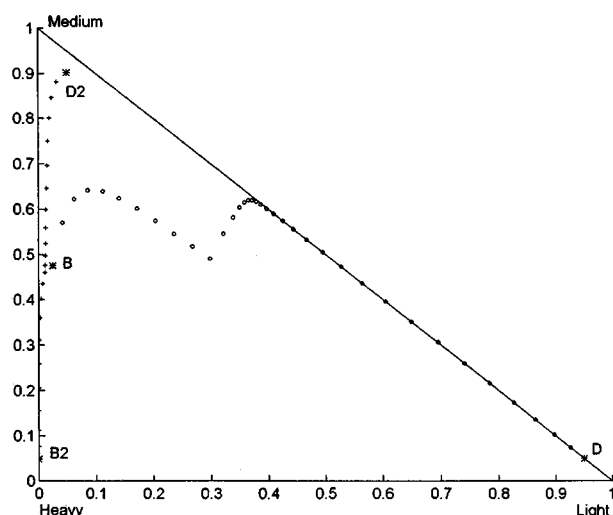


Fig. 7. Liquid composition in a conventional direct sequence two-column system at an actual number of trays.

reflux flow is needed for the same product specification. This is largely owing to the extra separation in the prefractionator.

The distance between feed composition and feed tray composition in Fig. 5 is much less than that in Fig. 7. This means that the FTCDC has less mixing in the feed stage than the conventional system. In the liquid composition variation of the conventional system as shown in Fig. 7, the composition of intermediate component is increased and decreased again from the feed tray to the bottom of the column. This indicates the remixing of the component in the first column of the conventional system. However, the remixing is not apparent in a prefractionator of the FTCDC. Both the feed mixing and the remixing of the intermediate component reduce the thermodynamic efficiency of the conventional distillation column.

A recent study [Agrawal and Fidkowski, 1998] indicates that the thermodynamic efficiency of the FTCDC is lower than that of a direct sequence arrangement of conventional distillation system for the particular ternary system of the system I of this study. The study utilizes the minimum work of separation for the computation of thermodynamic efficiency of an FTCDC. However, the irreversibility caused by the mixing at feed tray and the remixing of the intermediate component in the column of a conventional system is a main source of the reduction of the efficiency [Triantafyllou and Smith, 1992]. The conflicting outcome is yielded because of the omission of the irreversibility in the efficiency computation of the study [Agrawal and Fidkowski, 1998]. The irreversibility has to be considered in the computation of the thermodynamic efficiency of distillation systems.

For the comparison of operating cost between the FTCDC and a conventional distillation system, a similar design procedure to the proposed scheme is applied to a direct sequence two-column distillation system as explained earlier. The vapor boil-up rate for the first column of the conventional system is 590 mol/h and 350 mol/h for the second. Therefore, the conventional system requires 30% more heat duty. Although the number of trays in the conventional system has 11% less than the FTCDC, the cost of extra heat exchangers is much more than the extra tray cost. On the other hand, the high reboiler temperature of the FTCDC requires high cost steam.

Table 3. Investment and annual steam costs in dollars

	Petlyuk column	Conventional column	
		1 st	2 nd
Column	388,600	280,300	140,900
Tray	37,100	24,400	9,800
Reboiler	195,100	180,100	129,700
Condenser	322,100	300,700	230,200
Total investment	942,900	785,500	510,600
Steam	365,600	295,800	195,000

The reboiler temperature is higher than that of the reboiler of the first column in the conventional direct sequence distillation by about 11 °C found from the boiling point of mixture, but total energy cost of the FTCDC is less than that of the conventional system. When it is considered that high pressure steam costs 0.85% more per °C increased than low pressure steam [Douglas, 1988], the 30% reduction of heat duty is large enough to take care of the increased cost of high quality steam. For the numerical comparison of economics, investment and annual steam costs are calculated for the 100 kg-mole/hr of feed and listed in Table 3. The procedure and information of the economics is found from references [Douglas, 1988; Kim and Luyben, 1994], and the result indicates that the FTCDC has 27.3% saving in investment cost and 25.5% saving in steam cost over the conventional distillation system.

CONCLUSION

An approximate design procedure for fully thermally coupled distillation columns (FTCDCs) is proposed and implemented to example systems. The procedure gives a fast solution for a preliminary design, and eliminates difficulties encountered in the design of the FTCDC by using conventional design techniques, especially commercial programs, owing to the lack of information of interlinking streams.

The performance of the proposed design is proved from the design of three example systems. The analysis of the FTCDC is conducted with the help of the structural information, and the problem associated with the dividing wall construction, which is common practice in industry, is addressed. In addition, the detail of energy saving of the FTCDC is analyzed and some conflicting result from the previous study was found which does not count the irreversibility from the mixing in the feed tray.

ACKNOWLEDGMENT

Financial support from the Korea Research Foundation through Grant KRF-2001-002-E00124 is gratefully acknowledged.

NOMENCLATURE

- A : flow rate of component A in feed [mol/h]
- B : flow rate of component B in feed or bottom product [mol/h]
- C : flow rate of component C in feed [mol/h]
- D : overhead product
- F : feed

i	: component
L	: liquid flow rate [mol/h]
NC	: number of components
NF	: feed location
NP	: side product location
NR	: upper interlinking stage in a main column
NS	: lower interlinking stage in a main column
NT	: number of trays in a main column
NT ₂	: number of trays in a prefractionator
RP	: liquid split ratio
S	: side product
V	: vapor flow rate [mol/h]
VC	: vapor split ratio
x	: liquid composition [mol fraction]
y	: vapor composition [mol fraction]

Greek Letters

α	: relative volatility
β	: middle component split ratio
ϕ	: parameter in Eq. (5)

Subscripts

i	: component i
j	: component j
n	: tray number from bottom

REFERENCES

- Abdul Mutalib, M. I., Zeglam, A. O. and Smith, R., "Operation and Control of Dividing Wall Distillation Columns, Part 1: Degrees of Freedom and Dynamic Simulation," *Trans IChemE*, **76**, Part A, 308 (1998a).
- Abdul Mutalib, M. I., Zeglam, A. O. and Smith, R., "Operation and Control of Dividing Wall Distillation Columns, Part 2: Simulation and Pilot Plant Studies Using Temperature Control," *Trans IChemE*, **76**, Part A, 319 (1998b).
- Agrawal, R. and Fidkowski, Z. T., "Are Thermally Coupled Distillation Columns Always Thermodynamically More Efficient for Ternary Distillation," *Ind. Eng. Chem. Res.*, **37**, 3444 (1998).
- Annakou, O. and Mizsey, P., "Rigorous Comparative Study of Energy-Integrated Distillation Schemes," *Ind. Eng. Chem. Res.*, **35**, 1877 (1996).
- Carlberg, N. A. and Westerberg, A. W., "Temperature-Heat Diagrams for Complex Columns. 3. Underwood's Method for the Petlyuk Configuration," *Ind. Eng. Chem. Res.*, **28**, 1386 (1989).
- Cerda, J. and Westerberg, A. W., "Shortcut Methods for Complex Distillation Columns. 1. Minimum Reflux," *Ind. Eng. Chem. Process Des. Dev.*, **20**, 546 (1981).
- Chavez, C. R., Seader, J. D. and Wayburn, T. L., "Multiple Steady-State Solutions for Interlinked Separation Systems," *Ind. Eng. Chem. Fundam.*, **25**, 566 (1986).
- Douglas, J. M., "Conceptual Design of Chemical Processes," McGraw-Hill Book Co., New York, U.S.A., 569 (1988).
- Dünnebier, G. and Pantelides, C. C., "Optimal Design of Thermally Coupled Distillation Columns," *Ind. Eng. Chem. Res.*, **38**, 162 (1999).
- Fidkowski, Z. and Krolikowski, L., "Thermally Coupled System of Distillation Columns: Optimization Procedure," *AIChE J.*, **32**, 537 (1986).
- Glinos, K. N. and Malone, M. F., "Design of Sidestream Distillation Columns," *Ind. Eng. Chem. Process Des. Dev.*, **24**, 822 (1985a).
- Glinos, K. N. and Malone, M. F., "Minimum Vapor Flows in a Distillation Column with a Sidestream Stripper," *Ind. Eng. Chem. Process Des. Dev.*, **24**, 1087 (1985b).
- Glinos, K. N. and Malone, M. F., "Optimality Regions for Complex Column Alternatives in Distillation Systems," *Chem. Eng. Res. Des.*, **66**, 229 (1988).
- Gmehling, J., Onken, U. and Arlt, W., "Vapor-Liquid Equilibrium Data Collection," DECHEMA, Frankfurt/Main, Germany, Vol. I, Part 1, 2b and 6a, 562, 504, 649 (1980).
- Kim, Y. H. and Luyben, W. L., "Effect of Recycle on Chemical Reactor Controllability," *Chem. Eng. Comm.*, **128**, 65 (1994).
- Kim, Y. H., "Design of a Fully Thermally Coupled Distillation Column Based on Dynamic Simulations," *Korean J. Chem. Eng.*, **17**, 570 (2000).
- Kim, Y. H., "Structural Design of Extended Fully Thermally Coupled Distillation Columns," *Ind. Eng. Chem. Res.*, **40**, 2460 (2001).
- Kim, Y. H., "Structural Design and Operation of a Fully Thermally Coupled Distillation Column," *Chem. Eng. J.*, **85**, 289 (2002).
- King, C. J., "Separation Processes," 2nd ed., McGraw-Hill, New York, 235-237, 421 (1980).
- Lee, Y. S., Kim, M. G., Ha, D. M., Oda, A., Ito, C., Aragaki, T. and Mori, H., "Analysis of Packed Distillation Columns with a Rate-Based Model," *Korean J. Chem. Eng.*, **14**, 321 (1997).
- Lestak, F., Egenes, D., Yoda, H. and Hamnett, C., "Kellogg Divided Wall Column Technology for Ternary Separation," Proc. The 5th Int. Symposium on Sep. Tech. between Korea and Japan, 233 (1999).
- McCabe, W. L. and Smith, J. C., "Unit Operations of Chemical Engineering," 3rd ed., McGraw-Hill Book Co., New York, 568 (1976).
- Midori, S. and Nakahashi, A., "Industrial Application of Continuous Distillation Columns with Vertical Partition," Proc. The 5th Int. Symposium on Sep. Tech. between Korea and Japan, 221 (1999).
- Petlyuk, F. B., Platonov, V. M. and Slavinskii, D. M., "Thermodynamically Optimal Method for Separating Multicomponent Mixtures," *Int. Chem. Eng.*, **5**, 555 (1965).
- Seader, J. D. and Henley, E. J., "Separation Process Principles," John Wiley & Sons, Inc., New York, 510 (1998).
- Triantafyllou, C. and Smith, R., "The Design and Optimisation of Fully Thermally Coupled Distillation Columns," *Trans. IChemE*, **70**, Part A, 118 (1992).
- Underwood, A. J. V., "Fractional Distillation of Multicomponent Mixtures," *Chem. Eng. Prog.*, **44**, 603 (1948).
- Underwood, A. J. V., "Fractional Distillation of Multicomponent Mixtures: a Numerical Example," *Chem. Eng. Prog.*, **45**, 609 (1949).
- Wang, J. C. and Henke, G. E., "Tridiagonal Matrix for Distillation," *Hydrocarbon Process.*, **45**, 155 (1966).
- Wolff, E. A. and Skogestad, S., "Operation of Integrated Three-Product (Petlyuk) Distillation Columns," *Ind. Eng. Chem. Res.*, **34**, 2094 (1995).
- Yoo, K. P., Lee, K. S., Lee, W. H. and Park, H. S., "Diagnosis of Thermodynamic Efficiency in Heat Integrated Distillation," *Korean J. Chem. Eng.*, **5**, 123 (1988).