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Industrial Application of an Extended Fully Thermally Coupled Distillation Column to BTX Separation in a Naphtha Reforming Plant

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Abstract−Aromatic compounds are yielded from naphtha reforming in a petrochemical plant, and the products are separated with binary distillation columns for benzene, toluene, xylene and heavy components in sequence. In this study, the first three columns of the fractionation process in the naphtha reforming unit are replaced with an extended fully thermally coupled distillation column (EFTCDC) also known as the extended Petlyuk column. An industrial-sized application of the EFTCDC is examined to compare the performance of the column with a conventional system. From a structural design giving the optimum structure of the column, a practical column structure is derived and used in the HYSYS simulation to find the optimal operation condition for a given set of product specifications. The EFTCDC gives an energy saving of 9.7% over a conventional three-column process. In addition, it is proved that the design procedure is good for an industrial process of 18 components.

Key words: Process Design, Thermally Coupled Distillation, Fractionation Process, Multi-Component Distillation, BTX Separation

INTRODUCTION

Though fully thermally coupled distillation columns (FTCDCs) for the separation of a ternary mixture are actively implemented for various industrial applications in Europe [Amminudin et al., 2001] and Japan [Midori and Nakahashi, 1999], no practical application of an extended fully thermally coupled distillation column (EFTCDC) is reported yet. Like the FTCDC a significant energy saving from the EFTCDC is predicted, but the actual implementation of the column requires proper answers for the design and operation, which have been little studied. The EFTCDC replacing a conventional three-column system has one reboiler instead of three reboilers for the conventional system. A brief schematic diagram of the EFTCDC is shown in Fig. 1. There are three different arrangements of the EFTCDC [Sargent and Gaminibandara, 1976; Kaibel, 1987; Agrawal, 1996], and the combination of a main column and two satellite columns of the figure proposed by Agrawal [1996] has the best performance [Christiansen et al., 1997].

Most design procedures of the EFTCDC require iterative computation because of many degrees of freedom in the design and operation of the column. For instance, commercially available design packages begin with entering the structural information of the column, and the operational variables for a given set of product specification are yielded from design simulation. If the structural information is not known, a trial structure is repeatedly used for the simulation until the optimum column design is obtained. Therefore, a great deal of iterative computation has to be conducted to find the optimal structure.

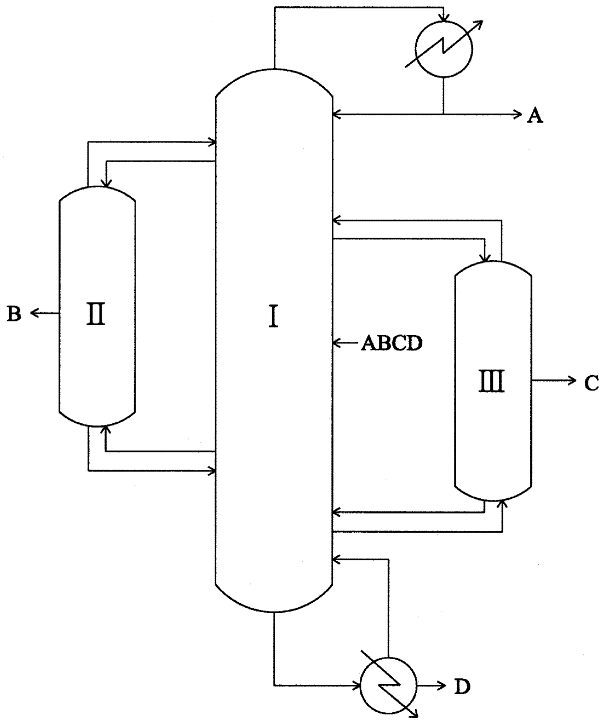

Fig. 1. Schematic diagram of an extended fully thermally coupled distillation column.

A simplified procedure to yield the optimal structure of an EFTCDC for the reduction of the computational burden has been proposed and applied to example systems [Kim, 2001b, 2002c]. The ideal structure of the minimum tray configuration is used to

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‡This paper is dedicated to Professor Hyun-Ku Rhee on the occasion of his retirement from Seoul National University.

construct a practical column system. The ideal tray distribution is adopted from the equilibrium distillation line, which has no mixing at feed tray and no remixing of intermediate components to maximize thermodynamic efficiency of the column. The structural information eliminates iterative computation with a commercial design procedure. Otherwise, the optimum structure has to be searched from the iterative simulation. The same procedure has been applied to the design of fully thermally coupled distillation columns [Kim, 2000, 2001a, 2002a; Kim et al., 2002b].

The fractionation process separates aromatic compounds from various streams, and its processing capacity is very large. For example, 135,000 barrels a day is processed at the fractionation process in Korea alone [KPIA, 2002], where about 2.9% of total world crude oil production is consumed [BP, 2001]. A series of binary-like distillation columns is used in the fractionation process, and each one of the columns produces only one purified product. By replacing the first three columns - separating BTX - in the process with an EFTCDC, an improvement of thermodynamic efficiency of the distillation system is available to result in the reduction of energy demand. The optimization of the process was studied for profit maximization [Chung et al., 1997]. Also, an optimum operating strategy of the system was searched in order to reduce energy demand [Lee et al., 2001].

In this study, the structural design procedure is applied to the design of an EFTCDC system to replace the first three columns of the conventional fractionation process in a naphtha reforming plant. For equilibrium computation and the design of operational variables, the commercial software HYSYS is implemented. The performance of the proposed system is compared with the conventional three-column system to examine usefulness of the new system and energy saving of the column.

STRUCTURAL DESIGN

From the design of a distillation column, two separate groups of information result: structural and operational design variables. Many procedures of distillation column design use limiting values of tray number and liquid flow, which are the basis of the column design. Other procedures not using the limiting values search the optimum design from direct minimization of the sum of investment and operating costs, but they require heavy computational load.

In this study, a design procedure beginning with the minimum tray structure is adopted for the design of an EFTCDC system. In total reflux operation, the required number of column trays is the minimum because the thermodynamic efficiency of the column is ideal. When the structure of a practical column is derived from the minimum tray column, the highly efficient column is yielded. In a multi-product distillation, if the liquid composition profile of a column is similar to one of residue curves, high thermodynamic efficiency is obtained since there is neither mixing at feed tray nor the remixing of intermediate components. The profile of residue curve is from ideal operation, and the minimum tray structure has the same profile of distillation line. Therefore, a practical column designed from the minimum tray has high efficiency.

In order to eliminate feed tray mixing, which reduces the column efficiency significantly [Kim, 2002a], it is assumed that the feed tray composition is equal to feed composition in the design of

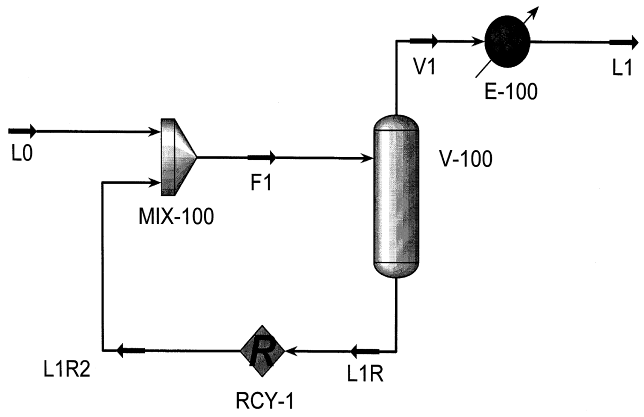

Fig. 2. An ideal separator for equilibrium calculation with liquid feed.

the minimum tray structure. Also, the structure has ideal tray efficiency, where the vapor composition of a stage is same as the liquid composition of one stage above. Hence, the design of the main column in Fig. 1 begins with the feed composition and the liquid compositions of the trays above the feed tray are evaluated from equilibrium relation in stage-to-stage computational manner. Assuming saturated liquid feed is provided, the liquid composition of the tray above the feed tray is calculated as

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

where K is an equilibrium constant.

In this study, however, 18 components are involved and so the equilibrium computation is not simple with an in-house calculation procedure. Therefore, a commercial design software HYSYS was used to find the equilibrium compositions. An ideal process with a simple separator is demonstrated in Fig. 2. Taking a small amount of liquid feed - say, 0.01 kmol/h - and a large amount of recycle - say, 1,000 kmol/h - gives an ideal equilibrium in the separator for a given pressure. In practice, a small variation of the numbers does not affect the calculated outcome, which indicates the computation at the process is not from material balance but equilibrium relation. The computed composition of vapor is given to the liquid feed composition of one stage above. This computation is readily carried out with the HYSYS and replaces the procedure of Eq. (1). The computation is repeated up to the top of the main column. The top produces benzene product here.

When the numbers of L0 and L1R are in near orders of magnitude, the computation in the flash tank (V-100) is carried out with material balance of inlet and outlet streams. However, if the L0 is intentionally set quite smaller than the recycle stream, the computation is done with the equilibrium relation. Though the component material balance gives exactly the same numbers between streams L0 and L1, taking L0 very small-less than the lower precision limit of L1R - yields the computation of L1 from the equilibrium relation. In this case some change of L1R does not affect the composition of L1 because the L1 composition is computed from the equilibrium at the flash tank, not from the material balance.

For the trays below the feed tray, the same procedure is applied. In this case, the feed composition is equal to the vapor composition

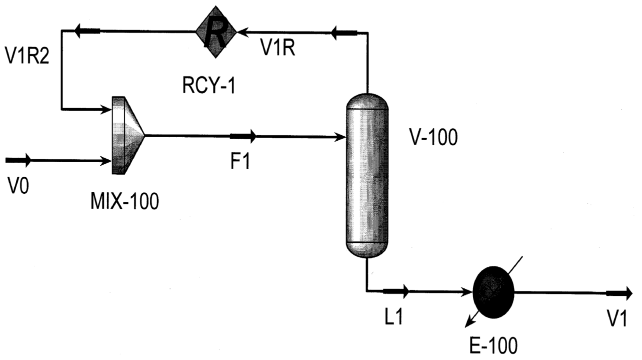

Fig. 3. An ideal separator for equilibrium calculation with vapor feed.

of one stage below the feed stage, and the liquid composition of the stage is obtained from the vapor composition by using the equilibrium relation, namely, the ideal HYSYS separator simulation. Again, computation proceeds successively down to the bottom. The bottom gives the heaviest product. Fig. 3 shows a stage of the computation with the HYSYS process. In the design of two satellite columns, computation begins with the composition of side products, and the whole process is employed in the same manner as the design of the main column.

The composition difference in the interlinking trays between the main column and two satellite columns produces irreversible mixing, which lowers the thermodynamic efficiency of the EFTCDC. Therefore, the compositions of the interlinking trays have to be close.

Table 1. Flow rates of feed and products in EFTCDC with unit of kmol/h

Component	Feed	Product			
		Overhead	Bottom	Side I	Side II
(Light)					
Benzene	87.850	86.986	0.0000	0.9431	0.0000
Dimethyl c-pentane	0.0120	0.0104	0.0000	0.0017	0.0000
(Intermediate I)					
Methyl c-hexane	0.0072	0.0000	0.0000	0.0073	0.0000
Toluene	338.10	0.0018	0.0001	336.43	0.7374
n-Octane	0.0489	0.0000	0.0000	0.0481	0.0005
(Intermediate II)					
Ethylbenzene	14.975	0.0000	0.0785	0.2850	14.516
p-Xylene	57.798	0.0000	0.5309	0.3336	56.601
m-Xylene	128.55	0.0000	1.2329	0.6629	125.96
o-Xylene	60.159	0.0000	1.5540	0.0631	58.447
n-Nonane	0.0064	0.0000	0.0001	0.0000	0.0062
(Heavy)					
n-Pentyl benzene	0.3303	0.0000	0.1812	0.0000	0.1541
Methyl-ethyl benzene	26.010	0.0000	22.830	0.0001	3.2150
tri-Methyl benzene	75.949	0.0000	76.084	0.0000	0.0011
Methyl-n-propyl bz	0.5701	0.0000	0.5706	0.0000	0.0000
di-Ethyl benzene	0.3303	0.0000	0.3307	0.0000	0.0000
o-Cymen	4.1197	0.0000	4.1258	0.0000	0.0000
tetra-Methyl benzene	4.7499	0.0000	4.7508	0.0000	0.0000
penta-Methyl benzene	2.2386	0.0000	2.2387	0.0000	0.0000

Table 2. Flow rates of feed and products in conventional system with unit of kmol/h

Component	Feed	1st		2nd		3rd	
		Overhead	Bottom	Overhead	Bottom	Overhead	Bottom
(Light)							
Benzene	87.850	86.958	0.8924	0.8924	0.0000	0.0000	0.0000
Dimethyl c-pentane	0.0124	0.0087	0.0037	0.0037	0.0000	0.0000	0.0000
(Intermediate I)							
Methyl c-hexane	0.0075	0.0000	0.0075	0.0075	0.0000	0.0000	0.0000
Toluene	338.10	0.0000	338.10	336.84	1.2588	1.2588	0.0000
n-Octane	0.0490	0.0000	0.0490	0.0480	0.0010	0.0010	0.0000
(Intermediate II)							
Ethylbenzene	14.975	0.0000	14.975	0.2152	14.760	14.749	0.0104
p-Xylene	57.798	0.0000	57.798	0.3022	57.496	57.300	0.1962
m-Xylene	128.55	0.0000	128.55	0.6102	127.94	127.44	0.4966
o-Xylene	60.160	0.0000	60.160	0.0708	60.089	57.229	2.8607
n-Nonane	0.0057	0.0000	0.0057	0.0000	0.0057	0.0056	0.0000
(Heavy)							
n-Pentyl benzene	0.3300	0.0000	0.3300	0.0000	0.3300	0.0863	0.2437
Methyl-ethyl benzene	26.010	0.0000	26.010	0.0002	26.010	2.8666	23.143
tri-Methyl benzene	75.950	0.0000	75.950	0.0000	75.950	0.0194	75.931
Methyl-n-propyl bz	0.5700	0.0000	0.5700	0.0000	0.5700	0.0000	0.5700
di-Ethyl benzene	0.3300	0.0000	0.3300	0.0000	0.3300	0.0000	0.3300
o-Cymen	4.1200	0.0000	4.1200	0.0000	4.1200	0.0010	4.1190
tetra-Methyl benzene	4.7500	0.0000	4.7500	0.0000	4.7500	0.0000	4.7500
penta-Methyl benzene	2.2389	0.0000	2.2389	0.0000	2.2389	0.0000	2.2389

Using the compositions of overhead and bottom products, the number of trays in the main column is found from the stage-to-stage composition calculation. Then, the liquid composition of trays above the side product in the satellite column II in Fig. 1 is computed tray-by-tray until a close composition with a stage of the main column is yielded. The same procedure is applied to the lower section of the satellite column. This process is also carried out for the satellite column III.

The molar flow rate of feed is given in Table 1. In addition, the specifications of products from the EFTCDC are listed in the table, and those of the conventional distillation system are summarized in Table 2. Though the feed is composed of 18 components, the design procedure handles only four components. Thus, the 18 components are separated into four groups of components according to the specification of products as indicated in the table. Minor components are grouped to the product having more amount of the component.

The outcome of the structural design for the minimum tray arrangement is shown in Fig. 4. The circles are of tray liquid compositions of the main column, and times symbols and pluses are of the satellite columns II and III, respectively. The circle marked with F is feed composition. The corners A, B, C and D represent benzene, toluene, xylene and heavy components, respectively. The times symbol close to corner B indicates that benzene is produced from the first satellite column, while toluene comes from the second. In the selection of interlinking trays, a close set of tray compositions of the main column and the satellite columns has to be determined. An exact match of the trays is not possible, and therefore the closest tray compositions are selected for the connection. The locations of feed tray and two side draws are readily found from the minimum tray structure by counting from the top of the columns. Because of high purity of the products, it is difficult to count the tray numbers from the figure, but it demonstrates the arrangement of the main and satellite columns and their liquid composition distribution.

Maintaining the minimum tray structure ensures the high thermodynamic efficiency of the minimum tray structure, which follows the profile of total reflux operation and has the highest efficiency.

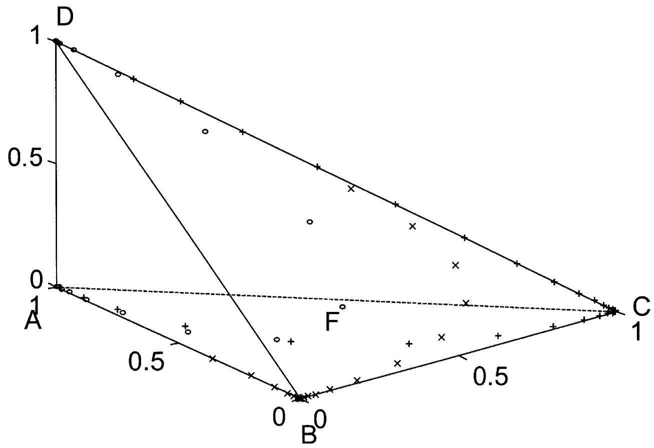

Fig. 4. Liquid composition profile of the EFTCDC in minimum trays. Circles are of main column, and times symbols of the first satellite column and pluses of the second satellite column.

The efficiency reduction is largely coming from mixing at the feed tray and remixing at the satellite columns [Triantafyllou and Smith, 1992], and the minimum tray structure does not have the source of the reduction. It is because the ideal structure has the composition of feed tray same as the feed composition, and the composition profiles of the main and satellite columns are similar to residue curves of the multi-component distillation system. By increasing the tray numbers in proportion from the minimum tray structure, the structure for the high thermodynamic efficiency is maintained. A factor of two in the expansion from the minimum tray structure to a practical column system is common in the industrial application [Seader and Henley, 1998]. This practice is also employed in the selection of feed tray location. Namely, the most commonly used rule to find the tray liquid composition close to liquid feed composition in the minimum tray structure [King, 1980] is used here. When the actual thermodynamic efficiency of each tray is the same throughout the column, the proportional increase of tray number does not alter the distillation line of the minimum tray distillation column and the location of feed tray. The locations of side draw and interlinking streams are not affected under the condition of even tray efficiency and the proportional increase of tray numbers. Therefore, the minimum tray structure is converted to a practical column with the factor and the result is summarized in Table 3. The last three columns show the tray numbers of a conventional three-column system to produce the same products as from the EFTCDC system.

OPERATIONAL VARIABLE DESIGN

In order to have products of a given specification, one needs a proper set of operation conditions for the distillation system of which the structure is found from the previous section. The condition is derived from a trial simulation until the computed product composition meets the specification. Because the commercial process design program HYSYS is used here, the trial computation with the known distillation structure is a relatively simple procedure. An illustration of the EFTCDC for quaternary separation in the HYSYS is shown in Fig. 5, which has the same structure given in Fig. 1. The schematic of the conventional three-column system is also demon-

Table 3. Structural design and operating condition

Name	EFTCDC			Conventional		
	Satt. I	Satt. II	Main	1st	2nd	3rd
Structural						
Number of trays	55	64	45	66	50	48
Feed/side product	18	28	26	33	25	24
Interlinking stages			13/35			
			11/39			
Operating						
Feed (kmol/h)			801.8	801.8	714.8	375.8
Overhead (kmol/h)			87.0	86.97	339.0	261.0
Bottom (kmol/h)			114.5	714.8	375.8	114.8
Side (kmol/h)	338.8	259.6				
Reflux (kmol/h)	763.9	682.9	2350.0	571.2	896.8	357.5
Vapor boilup (kmol/h)	400.0	603.3	1973.0	617.0	1133.0	553.6
Heat duty (GJ/h)			75.7	21.4	41.0	21.4

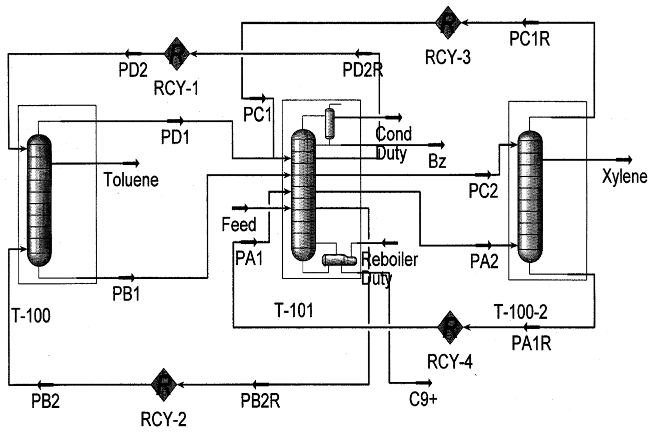

Fig. 5. Schematic diagram of an extended fully thermally coupled distillation column for quaternary separation.

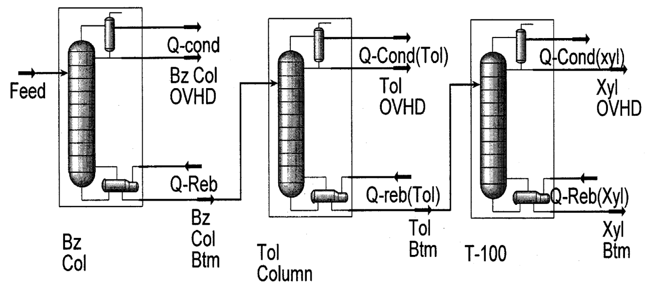

Fig. 6. Schematic diagram of a conventional coupled distillation system for quaternary separation.

strated in Fig. 6.

One of the benefits from the commercial program is that the equilibrium calculation for multi-component system is simple. In-house software needs the vapor-liquid equilibrium data that are not easy for the system of a large number of components. Design with the HYSYS requires the structural information of the distillation system, feed composition, flow rates of feed and products and column pressure. Except the structural information, others are given from the design project. Then, reflux flow is iteratively varied until the specified composition of product is yielded. Unless the components in feed formulate an azeotropic mixture, the proposed procedure works without any difficulty. The structural design procedure is based on the residue curves, and the pattern of the curves is similar in various multi-component systems except the azeotropic system.

In the design of distillation columns with the HYSYS, the information of column structure has to be determined at the initial stage. Then, operational variables are given to simulate the process and to examine the specification of products. The variables are adjusted until a predetermined product specification is found. In this regard, the design procedure of this study, which gives the structural information first, is suitable to the HYSYS design application. For example, a structural design technique for a fully thermally coupled distillation column using the three-column model was proposed by Triantafyllou and Smith [1992]; it requires matching the compositions of interlinking streams to result in time-consuming iterative computation. The proposed structural design of this study does not require the matching process to eliminate the computational load.

The HYSYS short-cut design procedure of a distillation column yields structural information, but it is only good for a conventional distillation system. The EFTCDC has interlinking streams of which compositions are not given to prevent from the application of the procedure. Therefore, a separate procedure to determine the structure of the EFTCDC is adopted from Kim [2001b, c]. Once the structure is determined, the formulation of the HYSYS model is simple and the model simulation continues until the desired products of given specification are obtained. The operational variables are found from the simulation result.

The step-by-step explanation of the proposed design procedure for an extended FTCDC is given below.

(1) Specify feed flow rate and compositions of feed and products.

(2) Perform stage-to-stage composition calculation for main and two satellite columns.

(3) Get tray numbers of main and two satellite columns and interlinking locations in minimum trays.

(4) Take twice the minimum as practical trays.

(5) Open HYSYS PFD widow and install two absorbers and one distillation column as shown in Fig. 5.

(6) Set the structural information of step 4 at the columns.

(7) Cut the recycle streams temporarily by giving dummy inlet name.

(8) Provide feed condition and composition.

(9) Put inlet side streams initial trial information. These are yielded from the minimum tray condition.

(10) Give trial liquid flow for each column and start simulation.

(11) If the simulation converges, connect the recycle streams one at a time.

(12) Check the product composition. If the composition is off from the specification, adjust the liquid flow rate until the specification is satisfied.

RESULTS AND DISCUSSION

An extended fully thermally coupled distillation (EFTCDC) system is applied to the fractionation process of a naphtha reforming

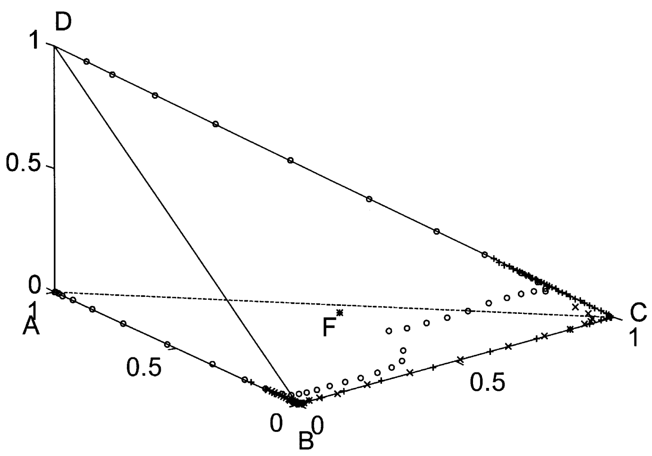

Fig. 7. Liquid composition profile of the EFTCDC in practical trays. Circles are of main column, and times symbols of the first satellite column and pluses of the second satellite column.

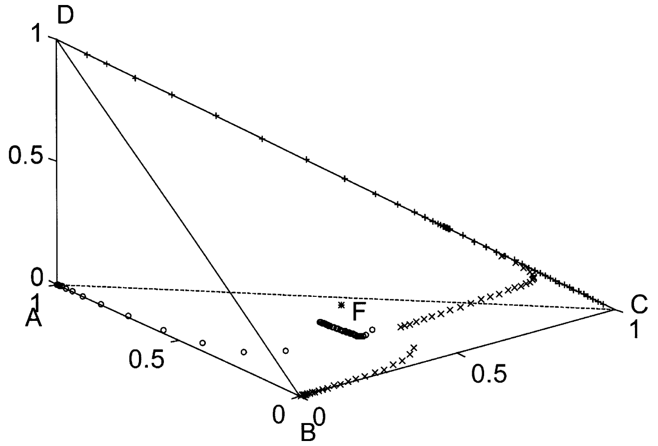

Fig. 8. Liquid composition profile of the conventional system in practical trays. Circles are of the first column, and times symbols of the second column and pluses of the third column.

plant as a major petrochemical process application of the energy saving distillation technique. The proposed design procedure is implemented for the processing of a given feed material of which molar flow rates are listed in Tables 1 and 2.

The design outcome of the EFTCDC system is summarized in Table 3 along with the result for a conventional three-column system. The table includes the information of the structural design and operational variables. The distribution of tray liquid composition for the EFTCDC is shown in Fig. 7, while that of the conventional three-column system is illustrated in Fig. 8. The corners of A, B, C and D denote the same components as in Fig. 4. The feed composition is indicated with the point marked F, and the distance between the point and the closest circle, which is feed tray, demonstrates the mixing at the feed tray. In Fig. 8, the large curvature of the liquid composition profile between the feed tray and bottom of the first column represents significant remixing of intermediate components in the lower section of the column. In addition, the distance between the bottom composition of the first column and the closest times symbol - the composition of feed tray in the second column - symbolizes the mixing at the feed tray. This mixing is found at the feed tray of the third column of the conventional system. However, the mixing is only found at the main column in case of the EFTCDC and the curvature indicating the remixing of the intermediate components is not significant here. From the liquid composition profiles, the thermodynamic efficiencies of the EFTCDC and the conventional three-column system are qualitatively evaluated.

For the performance examination between the EFTCDC and the conventional system, the heat duties of the EFTCDC and the conventional system are compared from Table 3, and some 9.7% less duty is used in the EFTCDC. For the same products from the same feed with the same number of total trays, less energy is necessary in the EFTCDC system as previous studies stated [Sargent and Gaminibandara, 1976; Kaibel, 1987; Agrawal, 1996; Christiansen et al., 1997]. Though the reboiler temperature in the EFTCDC is higher than that of the first and second columns in the conventional system and the steam for the reboiler may cost more, the same steam of intermediate pressure is used in both systems leaving no increase of the utility cost from the pressure increase. The same pressure group of steam as an intermediate pressure steam has the same price [Douglas, 1988]. Also, the reduction of heat duty lowers the investment cost for the construction of reboilers and condensers.

The EFTCDC has been proposed for the separation of a quaternary mixture, but it can be implemented in multi-component systems. The application of the EFTCDC to the first three columns of the fractionation process in this study indicates that the energy conservative system can be used in a variety of commercial processes not limited by the number of components.

CONCLUSION

A structural design procedure for an extended fully thermally coupled distillation system is implemented in the industrial-scale fractionation process of a conventional three-column system in a naphtha reforming plant. The commercial design software HYSYS is used in the computation of equilibrium tray compositions and operational variables.

The design outcome and performance comparison with a conventional system indicate that the proposed design procedure is useful to implement the EFTCDC for the industrial application involving much more than four components. The economics study shows the energy saving of 9.7% over the conventional tree-column distillation. In addition, the structural information found for the structural design is useful in the design of the EFTCDC with the commercial design program HYSYS.

ACKNOWLEDGMENTS

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NOMENCLATURE

A : benzene
B : toluene
C : xylene
D : heavier product
F : feed
K : equilibrium constant
x : liquid composition [mol frac.]
y : vapor composition [mol frac.]

Subscripts

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

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