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Design of a Fully Thermally Coupled Distillation Column for Hexane Process Using a Semi-Rigorous Model

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Abstract−An industrial scale hexane process is designed for the implementation of a fully thermally coupled distillation column (FTCDC). A semi-rigorous material balance and Peng-Robinson equilibrium relation are utilized in the structural design. The operational design is conducted with a commercial design program, the HYSYS. The design outcome of the structural design indicates it to be comparable with the practical system of a conventional two-column arrangement in field operation, which shows the effectiveness of the design procedure implemented here. The procedure is good for the system of many components found from actual field applications. In addition, an investigation of the energy requirement of the FTCDC and a conventional system shows that an energy saving of 34.1% is available with the FTCDC.

Key words: Thermally Coupled Distillation, Hexane Process, Structural Design, Petlyuk Column Design, Semi-Rigorous Model

INTRODUCTION

Although a thermally coupled distillation column (FTCDC) has been developed for the separation of a ternary mixture, it is industrially implemented for a multi-component system yielding three products of major components in a multi-component feed. Therefore, any two conventional distillation columns in series can be replaced with the FTCDC. An example of the application is given in Lee et al. [2003].

The minimum flow reflux flow rates of a main column and a prefractionator of the FTCDC have been calculated for the design of the column in many studies [Glinos and Malone, 1985; Fidkowski and Krolokowski, 1986; Carlberg and Westerberg, 1989], but commercial design software requires structural information instead of the operating condition in the process of the column design. Moreover, the FTCDC contains interlinking between the main column and prefractionator, which prevents one from implementing a conventional distillation design procedure to design of the column.

The three-column model was introduced in the design of an FTCDC by Triantafyllou and Smith [1992] and improved by including semi-rigorous material balance and equilibrium relation [Amminudin et al., 2001]. The main procedure of the design is to divide a main column into two separate columns for the elimination of interlinking.

On the other hand, the tray composition profile of equilibrium distillation is utilized in the structural design of an FTCDC for the determination of interlinking location and feed and side draw trays [Kim, 2001a, 2002b; Kim et al., 2002] and in the design of an extended FTCDC [Kim, 2001b, 2002a]. Because the equilibrium composition profile requires the minimum number of trays [Widagdo and Seider, 1996], a scaling factor of two is employed in the computation of a practical column. For the systems of highly non-ideal equilibrium relation, the structural resemblance between the minimum tray column and the practical column does not hold to generate design error from the scaling.

The hexane process separates hexane out of light naphtha produced from an atmospheric pressure distillation tower in a refinery. The product of the process is further treated for the removal of sulfur to be sold as a final product. As an industrial process the fractionation process in a naphtha plant has been investigated for energy saving [Lee et al., 2001, 2003; Kim et al., 2003], but the hexane process was not examined for this purpose.

In this study, a structural design procedure for the FTCDC was applied to the hexane process by using a semi-rigorous material balance and non-ideal equilibrium relation. The application procedure and economics of the new process and a conventional hexane process are explained in detail.

DESIGN PROCEDURE

An FTCDC is composed of a prefractionator and a main column as described in Fig. 1. When tray liquid compositions of the two columns are close to the residue curves of equilibrium distillation of a multi-component system, the thermodynamic efficiency of the distillation process is ideal and the previous design procedure [Kim, 2002] adopted the concept.

Though the tray composition profile similar to the residue curves is not obtained for a practical column unless the tray number is infinite, when feed tray composition is close to feed composition, near ideal efficiency is yielded.

The design of the prefractionator begins with the feed composi-

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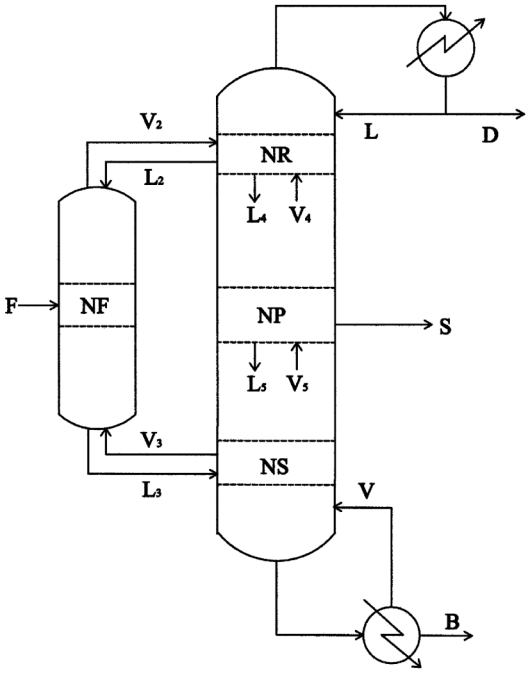

Fig. 1. Schematic diagram of a fully thermally coupled distillatioin column.

tion in order to make the feed tray composition close to feed composition listed in Table 1. In other words, the feed tray composition is assumed to be same to the feed. Then, the liquid composition of one stage above the feed tray is computed from the following material balance and the computation continues up to the top of the prefractionator.

$$x^{II}_{n,i} = (V_2 y^{II}_{n+1,i} - F z_i \gamma_{1,i}) / L_2 \quad (1)$$

where liquid and vapor flow rates are taken to be 1.5 times the minimum flow [Fidkowski and Krolikowski, 1986] and equimolal overflow assumption is applied. The actual flow rate is not the presumed value, but a common design guideline is implemented for design convenience. This will be discussed again later. The vapor composition in the equation is found from the Peng-Robinson equation with the parameters of the HYSYS database. Because the equilibrium calculation for 19 components of this study is not simple, a list of simplified composition is formulated with major components only, as in Table 2. The coefficient $\gamma_{1,i}$ is the transport ratio of component i through upper linking from the prefractionator to the main column, and it is readily calculated from the optimum split ratio β of intermediate component which is defined in Fidkowski and Krolikowski [1986]. The design parameters and the minimum flow rates are listed in Table 3.

In a similar manner, the vapor composition of the lower section of the prefractionator is calculated from the material balance beginning with the feed composition. Note that vapor composition is yielded instead of liquid composition unlike the upper section.

$$y^{II}_{n,i_{n,i}} = (L_3 x^{II}_{n-1,i} - F z_i \gamma_{2,i}) / V_3 \quad (2)$$

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

Component	Feed	FTCDC			Conventional 1st		2nd	
		Overhead	Bottom	Side	Overhead	Bottom	Overhead	Bottom
(Light)								
n-Butane	3.0316	3.0320	0.0000	0.0000	3.0315	0.0000	0.0000	0.0000
i-Butane	0.6517	0.6518	0.0000	0.0000	0.6517	0.0000	0.0000	0.0000
n-Pentane	26.040	26.051	0.0000	0.0000	26.040	0.0000	0.0000	0.0000
i-Pentane	13.479	13.484	0.0000	0.0000	13.479	0.0000	0.0000	0.0000
Cyclopentane	1.4812	1.4818	0.0000	0.0000	1.4811	0.0001	0.0001	0.0000
22-Methylbutane	0.2666	0.2664	0.0000	0.0002	0.2661	0.0006	0.0006	0.0000
2-Methylpentane	7.5840	6.9219	0.0022	0.6217	6.7074	0.8766	0.8765	0.0000
(Intermediate)								
3-Methylpenatne	5.0856	3.3096	0.0145	1.7302	3.1134	1.9722	1.9713	0.0009
n-Hexane	21.182	2.1110	1.3207	17.789	2.4825	18.699	17.791	0.9086
1-Hexene	0.0099	0.0077	0.0000	0.0021	0.0073	0.0026	0.0026	0.0000
Methylcyclopentane	2.6959	0.1196	0.6783	1.9189	0.1589	2.5369	1.8118	0.7251
(Heavy)								
Cyclohexane	1.7874	0.0043	1.4605	0.3136	0.0094	1.7779	0.0681	1.7099
Benzene	1.2541	0.0773	0.3239	0.8580	0.0965	1.1576	0.7982	0.3594
n-Heptane	8.0516	0.0000	8.0278	0.0224	0.0000	8.0516	0.0000	8.0516
2-Methylhexane	1.6330	0.0000	1.5957	0.0341	0.0000	1.6330	0.0000	1.6330
3-Methylhexane	1.3632	0.0000	1.3395	0.0218	0.0000	1.3632	0.0000	1.3632
Methylcyclohexane	1.2355	0.0000	1.2301	0.0051	0.0000	1.2355	0.0000	1.2355
Cycloheptane	1.1786	0.0000	1.1789	0.0000	0.0000	1.1786	0.0000	1.1786
Toluene	0.7385	0.0000	0.7382	0.0004	0.0000	0.7385	0.0000	0.7385
Total	98.750	57.519	17.910	23.318	57.525	41.224	23.320	17.904

Table 2. Modified flow rates of feed and products in kmol/h

Component	Feed	FTCDC		
		Overhead	Bottom	Side
(Light)				
i-Pentane	17.163	17.279	0.0000	0.0000
n-Pentane	35.372	34.587	0.0000	0.7999
(Intermediate)				
3-Methylpenatne	5.0854	2.9105	0.0036	2.1734
n-Hexane	23.888	2.6287	1.7032	19.551
(Heavy)				
n-Heptane	17.242	0.1150	16.203	0.7952
Total	98.750	57.520	17.910	23.320

Table 3. Design parameters and minimum flow

Item	Value
α_A	8.46
α_B	2.80
β	0.241
L_{1m}	57.7 kmol/h
L_{2m}	13.2 kmol/h

For the middle section of the main column between upper and lower interlinking trays, two material balances similar to Eqs. (1) and (2) are implemented. However, finding the interlinking trays requires an optimization procedure because the composition difference between two interlinking trays of the prefractionator and main column has to be as small as possible. An objective is formulated as

$$\underset{m,n}{\text{Min}}\sum_i \left|(x_{n,i} - x^{II}_{m,i})Fz_i\gamma_{1,i}\right| \tag{3}$$

where subscript m indicates tray number in the prefractionator and subscript n does tray number of the main column. Once the trays are determined, the liquid composition in the interlinking tray is yielded from the material balance.

$$x_{NR,i} = (V_4 y_{NR+1,i} + V_2 y^{II}_{1,i} - Fz_i\gamma_{4,i})/L \tag{4}$$

And, the tray liquid composition from the interlinking tray to the end of the main column is found in the same manner as above until the composition satisfies the specification of product.

$$x_{n,i} = (Vy_{n+1,i} - Fz_i\gamma_{4,i})/L \tag{5}$$

The stage-to-stage computation using the material balances gives tray numbers of the prefractionator and main column, feed and side draw location, and interlinking trays. While the numbers in the main column are implemented as computed, the numbers in the prefractionator have to be adjusted due to the assumption of feed tray composition. In this study, the counted numbers are multiplied by 1.7 using a common design guideline.

The outcome of the structural design is listed in Table 4. The numbers in parentheses are the computed results. In the beginning of the HYSYS simulation to find the operating condition for the specified products given in Table 1, the computed tray numbers were

Table 4. Tray numbers from structural design and operating conditions for the FTCDC and conventional two-column systems. Tray numbers are counted from top

Name	FTCDC		Conventional	
	Prefractionator	Main	1st	2nd
Structural				
Number of trays	29(7)	66(16)	25	70
Feed/side product	11(3)	32(8)	11	44
Interlinking stages		11(3)		
		57(14)		
Operating				
Feed (kmol/h)	98.75		98.75	41.22
Overhead (kmol/h)		57.52	57.53	23.32
Bottom (kmol/h)		17.91	41.22	17.90
Side (kmol/h)		23.32		
Reflux (kmol/h)	25.00	134.1	132.3	74.39
Vapor boilup (kmol/h)	94.00	169.3	175.7	89.92
Heat duty (GJ/h)		5.449	5.382	2.892

implemented, but the product composition was not available even with a large value of liquid flow. Considering that the tray numbers in a practical field process using a conventional distillation system are 36 and 100 for the first and the second columns, respectively, indicates that the computed tray numbers are too small to yield the given products. Therefore, the numbers are proportionally increased as given in Table 4. The error of the structural design is largely from inaccurate relative volatility and non-ideal relation of vapor-liquid equilibrium, which are used in the computation of design parameters listed in Table 3. One other source of the difference is that 5 major components instead of the actual 19 components are employed in the vapor-liquid equilibrium computation for simplicity. However, the column structure from the initial computation is applied in the modification, which gives a design basis of the practical distillation process.

With the determined structure, an HYSYS design project is formulated as illustrated in Fig. 2 and operating conditions are searched for the given products through the HYSYS simulation. Though some iteration with difference values of the operating conditions is conducted, yielding the outcome is a straightforward process. The sim-

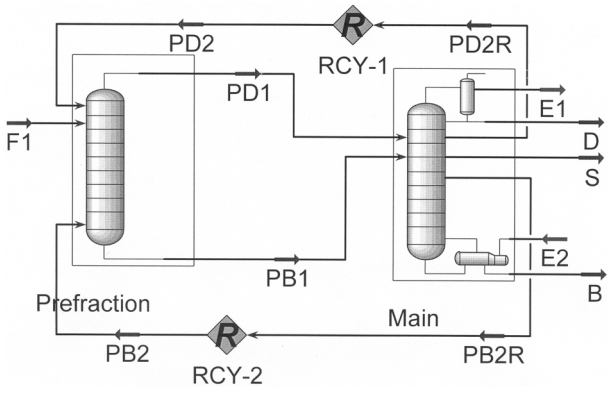

Fig. 2. HYSYS flow diagram of hexane process with a fully thermally coupled distillation column.

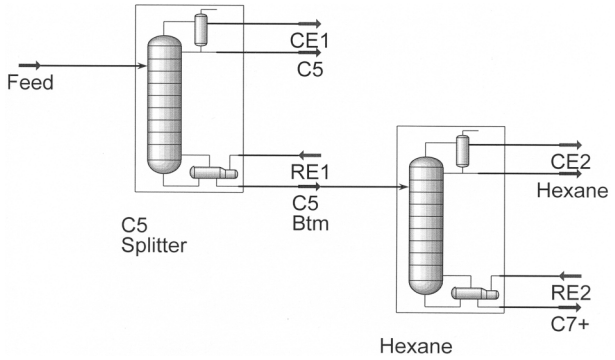

Fig. 3. HYSYS flow diagram of a conventional hexane process.

ulation result is listed in Table 4.

RESULTS AND DISCUSSION

The structural and operating information of the hexane process designed with the procedure presented above is shown in Table 4. For the comparison of the design outcome and energy consumption of the proposed FTCDC with a conventional hexane process, an HYSYS process is prepared as depicted in Fig. 3, which is a typical direct sequence distillation system and is practically implemented in field operation. The tray numbers and operating variables are listed in Table 4. Feed and product flow rates and specifications are the same for both systems. In addition, the total number of trays is set to be equal for economic evaluation. The tray numbers of 25 and 70 in the first and second columns of the conventional system are comparable to the practical tray numbers of 36 and 100 in field application when column efficiency of the practical system is considered.

In terms of energy requirement, the FTCDC consumes 34.1% less steam compared with the conventional system. Due to the less heat requirement, the investment cost of heat exchanger is also less by the same ratio while the construction cost of column is the same. The lower energy demand of the FTCDC indicates higher thermodynamic efficiency, which is explained with liquid composition profile of the systems. Fig. 4 demonstrates the profile of the FTCDC. The times symbols are of the prefractionator and the circles are of the main column. When the profile is compared with that of the conventional system given in Fig. 5, the distance between feed composition indicated with F and feed tray composition are quite different from each other. The times symbols in Fig. 5 denote the profile of the first column and the circles are of the second. The feed tray is represented with the middle crossing of two convex curves of the first column profile. The larger the distance is, the more the mixing at the feed tray is and the lower the efficiency is due to the irreversible mixing. In case of the conventional system, the feed tray mixing is observed in the second column too. The FTCDC has only one mixing at the feed tray in the prefractionator, in which the mixing is much less than that of the first column of the conventional system.

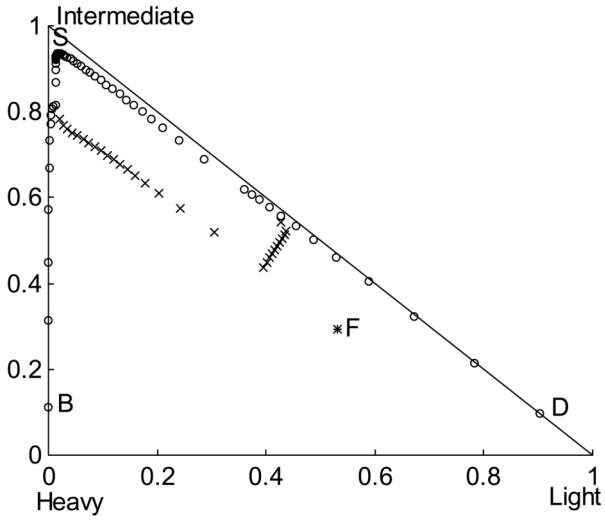

Fig. 4. Profile of tray liquid composition of hexane process with a fully thermally coupled distillation column.

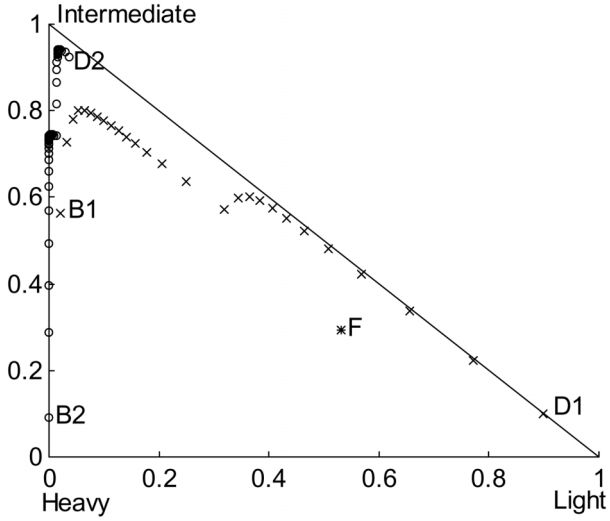

Fig. 5. Profile of tray liquid composition of a conventional hexane process.

Though the trays numbers of the FTCDC are increased by about 4 times from the initial computation, the computed base structure is not altered. The modification is induced largely from the simplified equilibrium computation and the error of relative volatility computation. Because the initial structural information is available, obtaining the practical structure from HYSYS simulation is much easier than the design without the structural information. In other words, the presented structural design here gives convenience in the design of a practical distillation system having many components in feed. In this case, 19 components are included, but the number does not incur much difficulty in the design process.

CONCLUSION

A structural design procedure of a fully thermally coupled distillation column is applied for the design of a hexane process having 19 components. The procedure utilizes a semi-rigorous material balance and adjusts the composition profile of the column to be close to the profile of equilibrium distillation for high column efficiency.

The design outcome indicates that the applied design procedure is effective for a practical distillation system having a large number

of components encountered in field applications. The structural information is comparable with that of the practical system currently operated in the field. The comparison with a conventional system for the same separation indicates that the FTCDC requires 34.1% less energy demand.

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NOMENCLATURE

B : bottom product
D : overhead product
F : feed flow rate [kmol/h]
L : liquid flow rate [kmol/h]
L_{1m} : minimum liquid flow rate in main column [kmol/h]
L_{2m} : minimum liquid flow rate in prefractionator [kmol/h]
NF : feed tray number
NP : side draw tray number
NR : location of upper interlinking tray
NS : location of lower interlinking tray
S : side draw
V : vapor flow rate [kmol/h]
x : liquid composition [mol fraction]
y : vapor composition [mol fraction]
z : feed composition [mol fraction]

Greek Letters

α : relative volatility
α_A : relative volatility of component A
α_B : relative volatility of component B
β : intermediate component split ratio
γ : transport ratio
$\gamma_{j,i}$: transport ratio of component i in section j

Subscripts

i : component
m : tray number
n : tray number

Superscript

II : prefractionator

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