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Approximate estimation of operational variables in fully thermally coupled distillation columns using pseudo-pinch points

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Abstract−An approximate procedure for the estimation of operational variables in fully thermally coupled distillation columns (FTCDCs) using two pseudo-pinch points of the feed and side draw trays is proposed, and its performance is examined with two example processes. The estimates from the proposed procedure show some 20% error compared with the results of rigorous simulation using commercial design software, the HYSYS. In addition, the relation between vapor flow rate and composition at one stage above the feed tray-required in the estimation of operational variables of the FTCDC-is analyzed to give information for the selection of the feed tray composition. A preliminary evaluation of operational variables helps to screen unrealizable design obtained often from iterative trial procedures employing the mathematical programming.

Key words: Distillation Column Design, Thermally Coupled Distillation, Pseudo-pinch Point, Operational Variable Estimation, Multi-component Distillation

INTRODUCTION

Though many short-cut design equations are available for the design of conventional distillation columns, the design of a fully thermally coupled distillation column (FTCDC) cannot utilize the equations due to the lack of information of the two-way interlinking between a prefractionator and a main column of the FTCDC. In the practical design of a conventional distillation column, operational variables such as reflux flow rate are determined first as design parameters, and then the structural design is followed based on the operational variables. This procedure is not applied to the design of the FTCDC, because it is difficult to find the operational information due to the unknown compositions of the interlinking streams. An estimation procedure of minimum liquid flow has been introduced by Fidkowski and Krolikowski [1], but it is not practical to use the flow rate in the FTCDC design because the minimum rate cannot give any information on the actual liquid flow rate.

Recent development of commercial design software for distillation columns has made the design of the FTCDC easy, because the software does not necessarily require compositions of the interlinking streams. Instead, a time-consuming, iterative trial computation has to be conducted, when the information of interlinking streams is not provided. As the application of thermally coupled distillation has been extended for many industrial processes [2], the problem of unknown interlinking information has become more significant in the design of the FTCDC. On the other hand, the structural design methods [3,4] for the FTCDC provide the information of column structure, such as number of trays, feed and side draw locations and interlinking trays reducing the computational load of the iterative trial design. A short-cut design [5], genetic programming [6] and new analyzing technique [7] have also been reported for the easy design of the FTCDC.

In an optimal distillation design the composition of feed tray is required to be close to feed composition in order to eliminate irreversible mixing at the feed tray. The mixing lowers the distillation column efficiency [8]. The determination of feed tray composition in the design of the FTCDC is less restrictive than that of a conventional distillation column, in which collinearity among the compositions of feed, overhead and bottom products has to be satisfied [9]. Because the feed stage composition is decided by vapor-liquid equilibrium and material balance, the match between feed and feed tray compositions is not simply manipulated by the column design. In a practical design some mismatch between feed and feed tray compositions is inevitable, and a pseudo-pinch point around the feed stage is formed to compromise the mismatch. This pseudo-pinch point can be utilized in the computation of operational variables of the FTCDC. Also, another pseudo-pinch point occurs at the tray of side draw as found from the composition profile of a main column. For the high purity product of side draw in the FTCDC, the column profile of the main column passes close to the vertex of intermediate component in the composition diagram, and a large number of trays are necessary for the separation near the vertex to form a pseudo-pinch point [10].

In this study, a unique distribution of column profile of the FTCDC having two pseudo-pinch points is employed in the formulation of material balances of a sectionalized FTCDC, and the balances are solved to estimate the operational variables of the FTCDC. The calculated vapor flow rates are compared with the results from the HYSYS simulation. In addition, the relation between vapor flow rate and feed tray composition is analyzed to help the selection of the composition for the optimal design of the FTCDC.

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COMPUTATION OF OPERATIONAL VARIABLES

A typical structure of the FTCDC is illustrated in Fig. 1, which consists of a prefractionator and a main column. For the derivation of the estimation equation of vapor flow rate in the prefractionator, the top section of the FTCDC was separated from the other as shown in Fig. 2. The separation points are determined by the fact that there are two pseudo-pinch points at the trays of feed and side draw. Whereas the tray of side draw is included in the section, the feed tray is not. The exclusion of the feed tray will be discussed below. At a pinch point in a distillation column the liquid and vapor compositions are the same, requiring an infinite number of trays for separation. Instead, at a pseudo-pinch point a low separation occurs to result in small variation of tray compositions as listed in Table 1. The composition profile was found from the HYSYS simulation of two example processes, of which the details are explained in the next section. As found from the table the vapor compositions of feed stage and one stage above feed tray are close, and therefore the former can be approximated from the liquid composition of one stage above feed tray and an equilibrium relation. This is why the feed tray is excluded from the separated section.

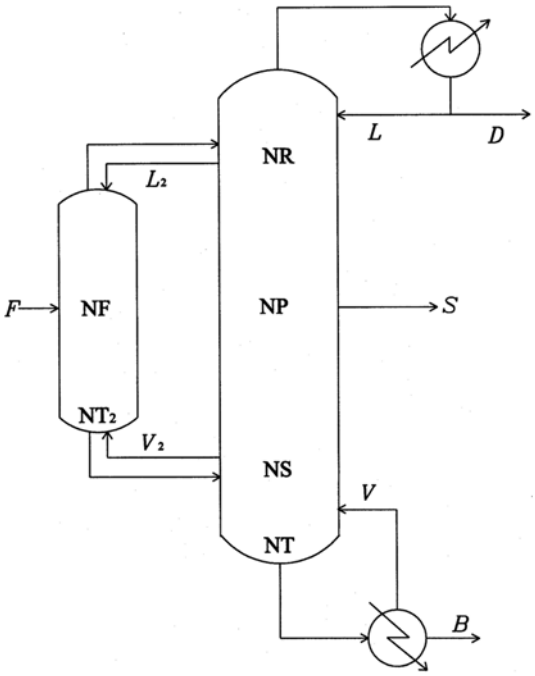

Fig. 1. A schematic diagram of a fully thermally coupled distillation column.

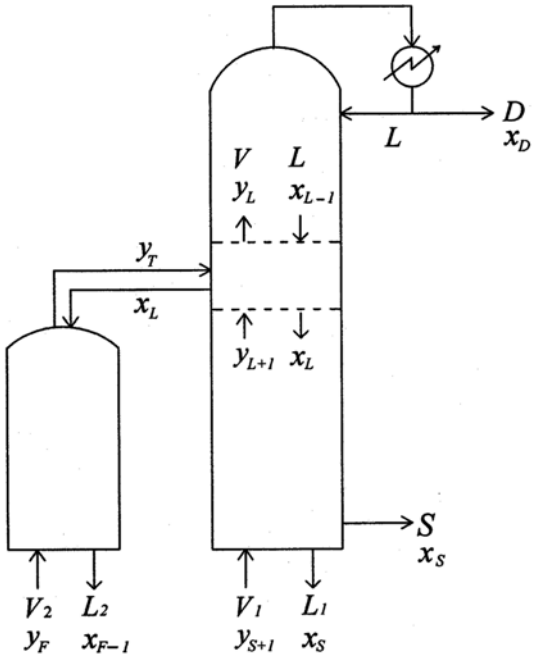

Fig. 2. A schematic diagram of top segment of the fully thermally coupled distillation column for the formulation of material balances calculating operational variables.

Table 1. Composition profiles found from the HYSYS simulation around feed, side draw and interlinking trays. The NF, NS and NL denote feed, side draw and interlinking trays, respectively. The superscripted vapor composition is computed from the equilibrium relation using the liquid composition. Tray numbers are counted from the top of the column

Stage	BTX			Butanol		
	x_A	y_A	y_A^*	x_A	y_A	y_A^*
NF-2	0.0938	0.2138	0.2121	0.2990	0.3845	0.3845
NF-1	0.0889	0.2115	0.2101	0.2859	0.3725	0.3725
NF	0.0846	0.2091	0.2083	0.2753	0.3630	0.3630
NS-1	0.0037	0.0079	0.0079	0.0272	0.0354	0.0354
NS	0.0037	0.0079	0.0079	0.0257	0.0334	0.0334
NS+1	0.0037	0.0079	0.0079	0.0244	0.0318	0.0317
NL-1	0.0470	0.0984	0.0965	0.5554	0.6303	0.6303
NL	0.0437	0.0918	0.0901	0.5069	0.5841	0.5841
NL+1	0.0239	0.0513	0.0503	0.4715	0.5486	0.5486

Material balances for the upper sections having boundaries at one stage above feed tray of the prefractionator and the side draw tray of the main column as demonstrated in Fig. 2 are given as

$$V_2 y_{F,A} - L_2 x_{F-1,A} + V_1 y_{S+1,A} - L_1 x_{S,A} = D x_{D,A} + S x_{s,A} \quad (1)$$

$$V_2 y_{F,C} - L_2 x_{F-1,C} + V_1 y_{S+1,C} - L_1 x_{S,C} = D x_{D,C} + S x_{s,C} \quad (2)$$

Note that the vapor compositions y_F and y_{S+1} can be estimated from the liquid compositions of one stage above the trays. For computational simplicity equimolal overflow assumption was employed here. The tray numbers are counted from the top of the column. Assuming that $x_{D,C}$, $x_{S,C}$, and $y_{S+1,C}$ in Eq. (2) are negligibly small gives the liquid flow rate in the prefractionator as

$$L_2 = V_2 y_{F,C} / x_{F-1,C} \quad (3)$$

The vapor flow rate in the prefractionator is found from Eqs. (1) and (3) with the neglected $x_{S,A}$, and $y_{S+1,A}$. Then,

$$V_2 = D x_{D,A} / (y_{F,A} - y_{F,C} x_{F-1,A} / x_{F-1,C}) \quad (4)$$

When the liquid composition at the one stage above the feed tray is given and the pseudo-pinch point assumption at the tray is applied, the vapor flow rate in the prefractionator is calculated from Eq. (4)

and the liquid composition is from Eq. (3).

All of component A is supplied through the interlinking tray of a main column, because the composition of the component A at the tray of side draw is negligible, meaning no production of component A through the tray. Therefore, material balances at the interlinking tray are formulated as below.

$$V - L = D \tag{5}$$

$$Vy_{L,A} - Lx_{L-1,A} = Dx_{D,A} \tag{6}$$

and

$$V_1 y_{L+1,A} - L_1 x_{L,A} = 0 \tag{7}$$

At the interlinking tray the vapor composition from one stage below and the liquid composition from one stage above are close, as listed in Table 1. Because there is a mixing due to the difference between vapor compositions of the top tray of the prefractionator and the interlinking tray, the distillation tray efficiency of the interlinking tray is low. Around the tray the vapor composition is close to the liquid composition of two stages above, and the tray efficiency is about a half of ideal efficiency. When the trial liquid composition at the interlinking tray is given, the vapor composition at the tray is computed from an equilibrium relation. Then, the liquid composition at one stage above the tray and the vapor composition at one stage below are computed by using the low tray efficiency explained above. Practically, the liquid composition of two stages above and vapor composition are the same. From the compositions the total vapor and liquid flow rates are calculated from Eqs. (5) and (6). Provided that the vapor and liquid flow rates in the prefractionator are known, the vapor and liquid flow rates, V_1 and L_1, at the middle section of the main column are computed to satisfy Eq. (7). Otherwise, the trial liquid composition is not valid. An iterative procedure of computation leads to the solution satisfying Eq. (7). Note that the composition of component C at the interlinking tray is negligible, leading to easy estimation of the liquid composition at the tray.

EXAMPLE PROCESSES

A benzene/toluene/m-xylene process modified from a practical BTX process [11] and a butanol process having a mixture of butanol isomers [12] were employed for the examination of the proposed estimation procedure of operational variables of the FTCDC in this study. Though the practical BTX process consisted of 18 components, three major components are adopted for the simplicity of computation. The composition and flow rates were derived from the original process. An equimolar mixture of 2-butanol/i-butanol/1-butanol system was used in the butanol process. The Peng-Robinson EOS was utilized for the vapor-liquid equilibrium calculation of the BTX process, and the UNIQUAC activity model was for the butanol process.

RESULTS AND DISCUSSION

To aid in the design of a fully thermally coupled distillation column, practical operational variables of the column were estimated by using the liquid compositions of pseudo-pinch points at the feed and side draw trays. For the examination of composition variation around the trays, HYSYS simulation was conducted with the specifications of feed and three products in two example processes as summarized in Table 2. The structural information of the FTCDC for the BTX and butanol processes is given in Lee, et al. [11] and Kim [12], respectively. The rigorous simulation results of tray liquid compositions in the example processes are found in Table 1. As listed in the table, the variations of liquid and vapor compositions around the feed and side draw trays are so small that the composition of a tray could be approximated from the composition of an adjacent tray. In addition, the compositions around the interlinking tray at the bottom three rows of the table show that the liquid composition of one stage above and the vapor composition of one stage below a tray are close. These are the basis of the development of estimation equations of operational variables in the previous section, and they are examined with the practical simulation results.

Table 2. Feed and product specifications. Units are in kmol/h

BTX	Feed	Overhead	Side	Bottom
Benzene	87.88	86.53	1.23	0.00
Toluene	338.12	0.42	334.47	2.74
m-Xylene	375.80	0.00	0.56	375.38
Total	801.8	86.95	336.26	378.12
Butanol	**Feed**	**Overhead**	**Side**	**Bottom**
2-Butanol	0.1	0.0975	0.0026	0.0000
i-Butanol	0.1	0.0021	0.0957	0.0024
1-Butanol	0.1	0.0000	0.0024	0.0973
Total	0.3	0.0996	0.1007	0.0997

Because there were some errors in the composition approximation and the equimolal overflow assumption was used, the estimation of operational variables had some discrepancy from the outcome of the HYSYS simulation. The estimated values from the proposed procedure of this study are listed in Table 3 with the rigorous simulation results using the HYSYS for the same feed and product specifications in two example processes. The composition of one stage above feed tray required in the estimation was adopted from the result of the HYSYS simulation. The estimation error compared with the rigorous simulation results ranges between 9% and 33%. When these values of the variables are used in the structural design of the FTCDC, some error in the number of trays estimated from the design may be generated. However, they can be good estimates for the trial values in the optimal design of the column. Other-

Table 3. Comparison of computed operational variables using the pseudo-pinch point procedure and the HYSYS simulation in the BTX and butanol processes

Variable (kmol/h)	BTX			Butanol		
	Pinch	HYSYS	Error (%)	Pinch	HYSYS	Error (%)
F	801.8	801.8		0.3	0.3	
V	1,703	2,001	−15	1.95	1.49	31
L	1,616	1,914	−16	1.85	1.39	33
V_2	492	538	−9	0.559	0.623	−10
L_2	245	347	−29	0.379	0.461	−18

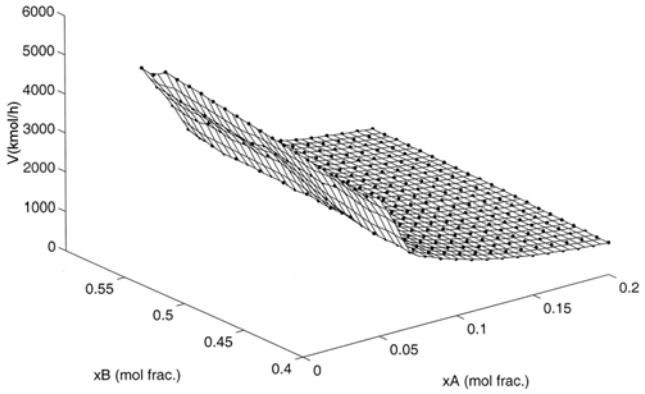

Fig. 3. Surface plot of vapor flow rates with different liquid compositions at one stage above feed tray in the BTX process.

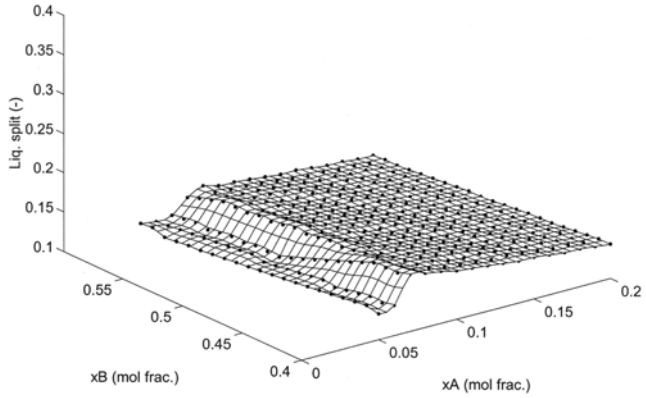

Fig. 5. Surface plot of liquid split ratio to the prefractionator with different liquid compositions at one stage above feed tray in the BTX process.

wise, numerous trials requiring a large amount of computation time are necessary in the design procedures utilizing mathematical programming.

In the estimation of vapor flow rate using Eq. (4) in the prefractionator, the composition of one stage above feed tray has to be provided. Though the feed composition can be an estimate of the tray composition, in a practical column the tray composition is different from the feed composition. The estimated vapor flow rates with various tray compositions in the BTX process are shown in Fig. 3. The composition increase of component A reduces the flow rate drastically, while the elevation of component B does mildly. The composition of component B at the feed tray is higher than that of the feed in a practical column [8]. A mixing-lowering the composition of component B-always occurs at the feed tray, which reduces the distillation column efficiency. If the composition of the component B in feed is higher than that in the feed tray, the efficiency will be raised from the mixing because the mixing helps the separation of the component B in the prefractionator. When the composition of one stage above feed tray is determined for the estimation of operational variables, this has to be considered. The same analysis of the relation between vapor flow rate and the tray composition was conducted in the butanol process as demonstrated in Fig. 4. Though

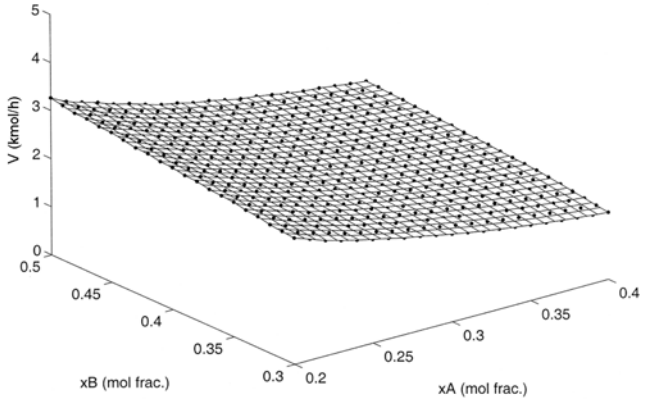

Fig. 4. Surface plot of vapor flow rates with different liquid compositions at one stage above feed tray in the butanol process.

less reduction with the increased composition of component A is observed, the pattern of variation is identical to that in the BTX process. The effect of the feed tray composition on the liquid split ratio, the portion of the liquid flow rate in the prefractionator to the total liquid flow, is illustrated in Fig. 5. No significant variation is observed in the split, because a large amount of liquid feed is supplied in the prefractionator and the liquid from the main column is small and has low effect on the separation.

Though a variety of optimization procedures utilizing the mathematical programming [13,14] can directly be implemented to obtain the optimal design of an FTCDC, they are time-consuming if no prior knowledge of operational variables is provided. In addition, many solutions from the procedure are not realizable in practical processes due to unbalanced vapor or liquid flow rate. For example, too large liquid flow for a given vapor flow induces weeping in a tray, lowering significantly the distillation column efficiency. In that case, the proposed procedure of this study helps to find if a design result is practical or not by estimating the operational variables in advance.

CONCLUSIONS

An approximate procedure for the estimation of operational variables in a fully thermally coupled distillation column using pseudo-pinch points was proposed here, and its performance was evaluated by applying to the BTX and butanol processes. The composition approximation at the points leads to simplified material balances in the estimation of the operational variables. The estimates using the proposed procedure showed some 20% error compared with the HYSYS simulation result. Also, the role of the composition at one stage above feed tray used in the estimation of vapor flow rate was investigated to give an estimation guideline of the composition. The proposed estimation of operational variables can help to examine the optimal design outcome from other design procedures.

ACKNOWLEDGMENTS

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NOMENCLATURE

D : overhead product flow rate [kmol/h]
F : feed flow rate [kmol/h]
L : liquid flow rate [kmol/h]
S : side product flow rate [kmol/h]
V : vapor flow rate [kmol/h]
x : liquid composition [mol frac.]
y : vapor composition [mol frac.]

Subscripts

1 : main column
2 : prefractionator
A : component A
C : component C
D : overhead product
F : feed
L : interlinking tray
S : side draw
T : top tray in prefractionator

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