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Structural design and operation of a fully thermally coupled distillation column

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Abstract

A rigorous structural design procedure for fully thermally coupled distillation columns (FTCDC) is applied to the example system of butanol isomers in order to show the design performance. The procedure gives structural information of the column, and therefore iterative computation encountered in the design using conventional procedure and commercial packages can be eliminated.

Using the outcome of the structural design, other topics, such as thermodynamic efficiency, dividing wall column structure and the arrangement of interlinking streams, are investigated. Finally, a 3×3 operation scheme, which has favorable indices of multivariable controllability, is examined by checking the control performances of set-point tracking and regulation with a model predictive control.

Keywords: Thermally coupled distillation; Petlyuk column design; Petlyuk column operation; Structural design; Multivariable control

1. Introduction

Though the design of operational information, such as the minimum reflux flow rate, in a fully thermally coupled distillation has widely been investigated, the structural design of the distillation column was rarely examined before. Since the fully thermally coupled distillation column (FTCDC), also known as the Petlyuk column [1], has interlinking between a prefractionator and a main column, usual multi-component design procedures are not applicable to the design of the column when the information of the interlinking streams is not given.

A design procedure to utilize the three-column model was introduced by Triantafyllou and Smith [2]. Separating the main column of the fully thermally coupled distillation system into two columns makes a system of three separate continuous distillation columns to which the short-cut design equations for the multi-component distillation design can be applied. Though the design procedure easily gives the tray numbers of the three separate columns, matching the compositions of interlinking streams requires adjustment and time-consuming iterative calculation.

On the other hand, using only the operation condition without the structural information leads to tedious iterative simulation in order to find a proper structure of the column. This problem also arises when the commercial design program, e.g. HYSYS, is utilized. Moreover, an inadequate structure does not give a converged solution in the process of simulation for the design.

For the simplicity of column construction, a dividing wall structure is preferred and has been adopted in many studies [3–6]. But the structure adds the complexity in the design since the number of trays in a prefractionator has to be same or close to the tray number in the middle section of a main column. Another problem associated with the dividing wall structure is that controlling the split of liquid and vapor flow is difficult.

Agrawal and Fidkowski [7] showed that the thermodynamic efficiency of fully thermally coupled distillation is not so high as suggested in earlier studies for some cases. The thermodynamic efficiencies computed from minimum work of separation and energy loss of a conventional system and the fully thermally coupled distillation are compared in the study. Yet the improvement of the efficiency in the coupled system is largely due to the less mixing in feed stage and remixing of middle component in a prefractionator [2], and the mixing and the remixing are not counted in the study.

When the compositions of feed and liquid in feed tray are different, the introduced feed is mixed with the tray liquid and the mixing causes irreversibility to decrease the thermodynamic efficiency. In the first column of a conventional ternary separation system in direct sequence, the composition of intermediate component in the middle of the column

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Nomenclature

B	flow rate of bottom product (mol/h)
D	flow rate of overhead product (mol/h)
F	flow rate of feed (mol/h)
h	liquid enthalpy (kcal/mol)
H	vapor enthalpy (kcal/mol)
K	equilibrium constant
L	reflux flow rate (mol/h)
L_2	liquid flow rate in a prefractionator (mol/h)
L_D	liquid flow rate in a main column (mol/h)
M	liquid holdup (mol)
NF	feed tray number
NP	side draw tray number
NR	location of upper side stream
NS	location of lower side stream
NT	number of trays in a main column
NT_2	number of trays in a prefractionator
S	flow rate of side product (mol/h)
t	time (h)
T	tray temperature (°C)
V	vapor flow rate (mol/h)
V_2	vapor flow rate in a prefractionator (mol/h)
V_B	vapor boil-up rate (mol/h)
x	liquid composition (mole fraction)
y	vapor composition (mole fraction)
z	feed composition (mole fraction)

Subscripts

B	bottom product
D	overhead product
i	component
j	component
n	tray number from the bottom
S	side product

is higher than that of bottom product because its distillation line is convex. Unless feed has high concentration of the intermediate component, the composition of the component goes up and down along with trays from feed tray to the bottom of the column. In other words, the intermediate component is refined first and then mixed with others while tray liquid flows down the column. This is called remixing and its irreversibility reduces the thermodynamic efficiency.

The operational complexity of an FTCDC has prevented from the wide utilization of the column ever since it was introduced a half century ago. Since a main column and a prefractionator are interlinked, more degrees of freedom than two binary distillation columns are involved and they are five at steady state [8]. There are not enough manipulated variables to formulate control loops equivalent to the degrees of freedom, and therefore multiple steady-state solutions are obtained for a given set of product specifications.

By rearranging sections in a main column and a prefractionator, various configurations of an FTCDC for the easy manipulation of vapor flow between the main column and a prefractionator are proposed by Agrawal and Fidkowski [9]. The pressure difference between the main column and prefractionator has a key role to determine a plausible alternative.

Rigorous simulation models associated with mathematical optimization are utilized to find the optimal design and operational condition for multi-product distillation systems [10]. However, the procedure gives a local minimum solution because of the mathematical limitation of the optimization technique.

In order to alleviate the control difficulty of an FTCDC, the reduction of the number of interlinking streams is attempted by installing a heat exchanger at the interlinking streams [11]. The proposed structures provide energy saving comparable to the fully thermally coupled system in some cases. Wolff and Skogestad [12] examined possible control schemes of the column and suggested that controlling the tray temperature close to the most critical composition measurement gives better performance than the direct composition control. In a dividing wall distillation column, cross pairing control structures are suggested and the role of liquid and vapor splits is investigated by Abdul Mutalib and Smith [4].

In this study, a structural design procedure for fully thermally coupled distillation columns is explained with an example system having three different feed compositions. The thermodynamic efficiency and multiple design solutions associated with the FTCDC are examined. The effect of the mixing in feed tray and the remixing of middle component in a prefractionator is examined using the liquid composition profiles. In addition, a 3×3 control scheme is utilized for the operation of the column, and its control performance with a model predictive control is investigated.

2. Structural design

A brief schematic diagram of FTCDC is shown in Fig. 1. Since there are two interlinking streams between a prefractionator and a main column, the conventional multi-component column design procedure is not directly implemented unless the compositions of the interlinking streams are given. But, none of previous studies gives the compositions without an iterative computation.

Using the three-column model [2], a short-cut design procedure for the conventional multi-component distillation can be utilized in the design of an FTCDC. In the three-column model, a main column is divided into two columns separated at the tray of side draw. In this case, it is required to match the compositions entering and leaving streams of the bottom tray of upper section and the top tray of lower section of the two separate columns, which leads to tedious iterative adjustment. In addition, since an ideal equilibrium is assumed between the vapor and liquid of interlinking streams and the short-cut design equations of multi-component distillation

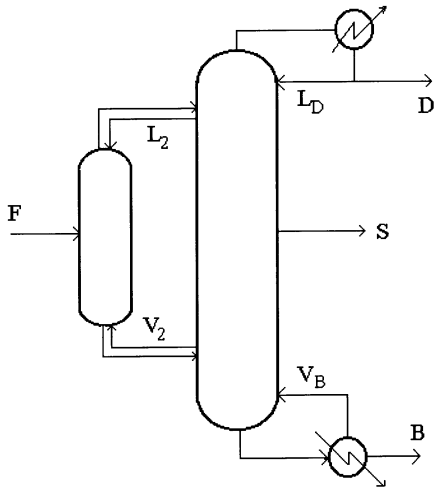

Fig. 1. Schematic diagram of a fully thermally coupled distillation column.

columns are employed in the design, the outcome is not accurate enough to be implemented as the initial condition for a rigorous simulation.

Unlike a binary system, in a ternary distillation, there are many distillation lines to connect the same composition of overhead and bottom products depending upon vapor boil-up rate, and the composition in the middle of the lines is quite different from one to another. Thus, when a composition in the middle of a distillation line is given, the path of a ternary distillation line is set. In a main column of fully thermally coupled distillation, the composition of side product is equal to the composition of the stage of the side draw. Namely, the composition profile of the main column with total reflux operation and the assumption of ideal tray efficiency, is readily obtained using the stage-to-stage computation. For computational purpose, a very large reflux flow is used instead of the total reflux.

For the side product is drawn from a main column, the design of the column begins with the composition of the product. Starting at the stage of side product, the liquid composition at one stage above the product stage is computed using the composition of the product and an equilibrium relation:

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

where $K_{n,i}$ is an equilibrium constant of the ith component at the nth tray from the bottom and obtained from an equilibrium relation. This procedure continues until the tray composition meets the specification of overhead product. The liquid composition of the stages below the side product stage is found in the same manner and the composition equation is modified as Eq. (2):

$$x_{n-1,i} = \frac{x_{n,i}}{K_{n-1,i}\sum_j (x_{n,j}/K_{n-1,j})} \quad (2)$$

Here, the equilibrium constant, K, has to be calculated iteratively because the composition used in the equilibrium relation is unknown, but the computation procedure is simple. Again, this stage-to-stage calculation continues until the liquid composition satisfies the specification of bottom product.

The same procedure is applied to the design of a prefractionator with the assumption that the composition of feed stage is equivalent to feed composition. In this case the end stage composition is not determined yet, and therefore the computation continues in a similar manner as in the main column design.

Now, the interlinking stages between the main column and the prefractionator are decided by matching the composition of top and bottom trays of the prefractionator and their correspondent trays in the main column. For an exact match between them is unlikely, the closest match is found to determine the interlinking trays. The closer the match between the concentration of top and bottom of a prefractionator and a main column is, the better the design is. Therefore, the trays of the smallest difference have to be selected.

In the process, however, there is one thing to be considered. A small amount of the third component, e.g. the heaviest component in the upper interlinking, is practically transferred from the prefractionator to the main column and the trays between upper interlinking stage and top tray are necessary to eliminate the component from the product. The same processing is required in the trays between the lower interlinking stage and bottom tray of the main column. This removal of the third component has to be considered in the selection of the interlinking stages. The location of feed and side product stages is directly obtained from the stage-to-stage calculation.

The resulted design gives the minimum number of trays, since the design is conducted for a total reflux operation. In many field applications, twice the minimum number is employed as an actual tray number [13]. Therefore, the actual number of trays of an FTCDC system is taken to be twice the calculated minimum. The optimality of this practice can be checked comparing the required reflux flow for different number of multiplying factor. A previous study [14] indicates that the factor of two is reasonable for practical application. The locations of feed and side product stages and interlinking stages are also determined by taking twice the stage numbers in the minimum design.

The proposed design procedure here is quite different from the conventional design in terms of determining column structure, such as the number of trays and location of feed. In the conventional design, the minimum liquid flow is calculated first and an optimum liquid flow is decided to find the structural information. However, the same procedure is unable to be implemented to the design of an FTCDC unless the information of interlinking streams is given. This is the main reason to utilize an alternate procedure here; structural design first.

3. Operational design

The analysis of degrees of freedom by Abdul Mutalib and Smith [4] indicates that there are nine manipulated variables for the operation of an FTCDC. In the steady-state design, the flow rates of three products are fixed and so are the feed temperature and column pressure. Therefore, four of reflux flow, vapor boil-up, liquid split from a main column to the top of a prefractionator and vapor split from a main column to the bottom of a prefractionator have to be determined from the operational design.

Many previous studies [15–17] examined the minimum liquid flow of a prefractionator and a main column using the Underwood equation [18,19]. The optimum liquid split is also given in the studies. However, an actual liquid flow is not given in the studies. The flow is numerically found from simulation. Referring to the minimum liquid flow and the optimum split, an actual liquid split ratio is yielded. Vapor split ratio is readily found from the steady-state material balance. Therefore, the liquid and vapor flow rates are unknown design variables, and they are numerically searched for the given specification of products.

The steady-state material and energy balances along with the UNIQUAC equilibrium relation are utilized in the evaluation of the product composition. Note that the structure of the FTCDC is known. In this process, the optimum liquid split has to be checked if it is true optimum, because the predicted minimum is too conservative [20]. For the example systems of this study, the predicted split is not the optimum and new optimum split is numerically looked for. The new optimum split is searched from examining if the reflux flow is the lowest while the composition of products meets the given specification.

The design specification includes feed flow rate, feed composition and composition of overhead, bottom and side products. The itemized design procedures are listed as follows:

1. Specify F, z_i, x_D, x_B and x_S.
2. Perform stage-to-stage composition calculation.
3. Get NT, NT_2, NF, NP, NR and NS in minimum trays.
4. Take twice the minimum as practical trays.
5. Assume liquid split ratio.
6. Provide L_D and V_B and calculate L_2.
7. Find L_n and V_n using equimolal overflow assumption.
8. Assume linear composition profile to calculate initial $x_{n,i}$.
9. Compute equilibrium constant with the UNIQUAC equation.
10. Obtain new $x_{n,i}$ using matrix inversion.
11. Calculate h_n and H_n.
12. Compute V_n from energy balances.
13. Obtain L_n from material balances.
14. If the total ΔT_n is greater than limit, go to step 9.
15. If product compositions do not meet the specification, adjust L_D and V_B and go to step 6.
16. Check L_D minimum. If not, go to step 5.
17. Stop.

4. Dynamic simulation

In order to analyze the operational characteristic of an FTCDC, its dynamic simulation is conducted in which the change of operation variables is applied and examined the variation of product composition. The initial operation condition of the dynamic simulation is derived from the design result of the previous section.

The liquid composition is updated from the material balance of a component in a tray:

$$M_n \frac{dx_{n,i}}{dt} = L_{n+1}x_{n+1,i} + V_{n-1}y_{n-1,i} - L_n x_{n,i} - V_n y_{n,i} \quad (3)$$

where the initial value of the liquid holdup, M_n, is derived from liquid flow rate using the Francis weir equation [21]. Unless the initial liquid flow rate found from the rigorous design of the previous section is accurate, the initial steady state of the dynamic simulation is not attainable. Therefore, the outcome of the design has to be very accurate. The high non-linearity contained in the Francis weir equation causes the problem associated with the initial convergence of the dynamic simulation.

Vapor holdup in a tray is ignored, since its amount is much less than liquid holdup. Vapor flow rate is computed from energy balance in a tray, and liquid flow rate is from material balance. The UNIQUAC equation is employed in the evaluation of equilibrium composition.

5. Example system

The proposed design procedure of this study does not utilize short-cut design equations, so a generalized design outcome of ideal ternary systems having an equilibrium relation with relative volatility is not delivered here. The system is a ternary system of *s*-butanol–*i*-butanol–*n*-butanol. It is an alcohol system having near ideal equilibrium.

Three different feed materials are an equimolar mixture (F1) and two mixtures of mole fractions of 0.75–0.125–0.125 (F2) and 0.125–0.75–0.125 (F3). In the selection of feed composition, it is presumed that the impact of high concentration of the lightest component in feed on the column design is similar to that of the heaviest component.

The design specification of products in the example system is set to 0.9 of mole fraction of the middle component in side product, 0.95 of the lightest component in overhead product and 0.95 of the heaviest component in bottom product. For equimolar feed, the fractional component recovery is same to the product specifications. In the case of feed F2, the component recoveries of the lightest component in overhead product, middle component in side product and heaviest component in bottom product are 0.99, 0.64 and 0.96, respectively. With feed F3, the numbers are 0.68, 0.99 and 0.68 for the example system.

Table 1
Design result of an example ternary system

Feed	NT	NT_2	NS	NR	NF	NP	L	V	L_2
F1	72	20	10	57	9	31	960.8	1006.5	325.0
F2	72	20	6	63	15	31	611.7	803.0	349.3
F3	72	20	16	45	11	31	660.1	650.7	166.4

6. Design results

The design outcome of the example system using the proposed procedure is listed in Table 1. The table includes the numbers of trays in a prefractionator and a main column and location of interlinking, feed and side product trays. Also, the operational information of reflux flow and vapor boil-up rates and the liquid flow rate in the prefractionator is contained. The feed flow rate is 300 mol/h for all the cases.

The liquid composition in trays for the system with equimolar feed is illustrated in Fig. 2. The numbers in the figure are tray numbers, and the mid-section means the trays between upper and lower interlinking stages of a main column. The circles are of a main column and the plus symbols are of a prefractionator. Note that the distance between the point F, the feed composition, and the closest point, the feed tray composition, denotes composition difference and the magnitude of mixing at the feed tray. The mixing has the most significant effect on the thermodynamic efficiency of the system. In addition, the decrease of the concentration of intermediate component in the lower section of the prefractionator demonstrated by the curvature between the feed tray and the bottom, indicates the remixing of the component to reduce the efficiency.

7. Thermodynamic efficiency

While the distillation lines of a conventional two-column system for ternary separation has quite different pattern compared with the residue curve of the ternary system, a fully thermally coupled system has similar one. It means that the fully thermally coupled system has less mixing and remixing in the distillation process. Mixing is an irreversible process, and its reverse process, separation, and requires a certain type of energy. Therefore, it reduces the thermodynamic efficiency of a process having the mixing.

The thermodynamic efficiency of a fully thermally coupled distillation is higher than that of a conventional distillation in the separation of a ternary mixture. In the study of Agrawal and Fidkowski [7], the thermodynamic efficiencies of the conventional system and the fully thermally coupled distillation are examined by including energy loss in the computation of the efficiencies. Since heat is supplied at the highest possible temperature in the fully thermally coupled distillation system, energy loss is larger than the conventional system. However, the amount of heat requirement in the fully thermally coupled system is much less than that of the conventional system, and the total utility cost adjusted for the high price steam used in the coupled system is less than the conventional system [14].

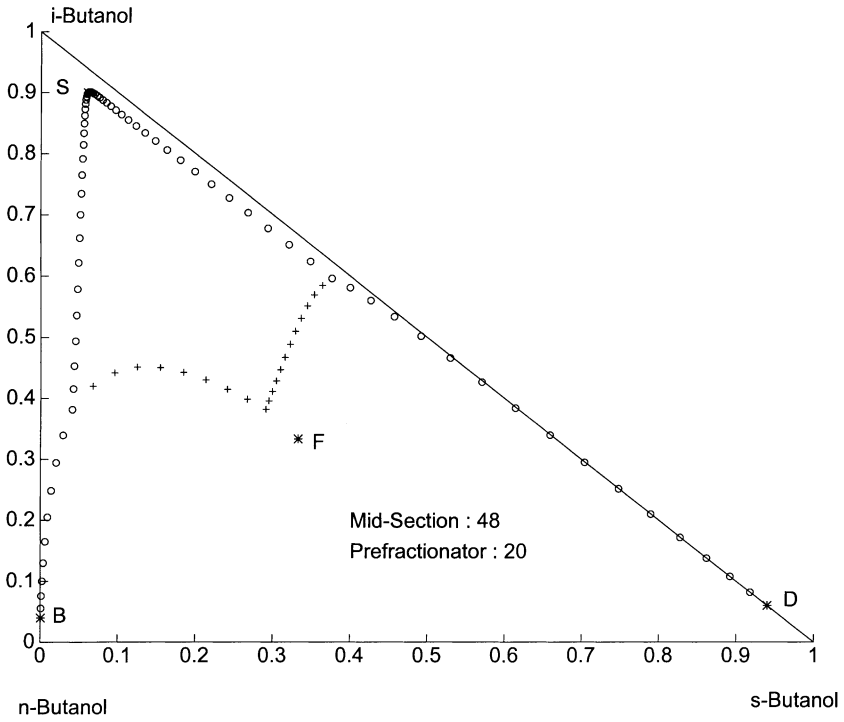

Fig. 2. Liquid composition in a fully thermally coupled distillation system with 48 tray mid-section and 20 tray prefractionator.

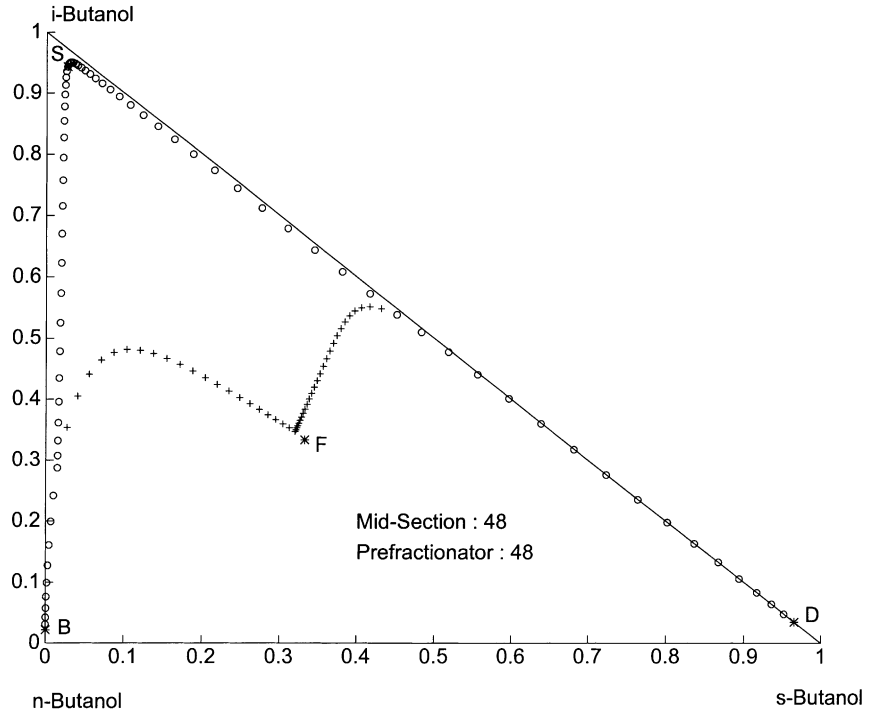

Fig. 3. Liquid composition in a fully thermally coupled distillation system with 48 tray mid-section and 48 tray prefractionator.

Triantafyllou and Smith [2] explained that the remixing of middle component in a conventional distillation and the mixing in feed tray induce the thermodynamic irreversibility to result in the efficiency reduction. In order to evaluate the effects of the remixing and the mixing in feed tray in separate, various combinations of tray numbers in a prefractionator and the middle section (between upper and lower linking stages) of a main column are examined. The combinations are arranged from the initial structural design of the base system.

When 28 trays are added to the prefractionator of the system to make the same number of trays (48) of a prefractionator and the middle section of a main column and the same amount of reflux flow is provided, the liquid composition profile is given in Fig. 3. The added trays are distributed proportionally from the structure of the prefractionator in the base system. The composition profile between the feed tray, the closest tray to the feed composition, and bottom tray of the prefractionator shows the remixing of middle component. The peak of the profile is the highest concentration of intermediate component and the concentration diminishes as moving from the peak to the bottom of the prefractionator. In other words, the higher the curvature is, the more the remixing is. The mixing in feed tray is simply found from the distance between the feed composition and the feed tray composition. Notice that by adding the 28 trays the numbers of trays in a prefractionator and the middle section of a main column are the same and the construction of dividing wall structure is available.

Table 2
Reflux flow rates for same product with different column structures

Mid-section	NT_2	Sum	Reflux flow
48	20	68	960.8
48	48	96	831.6
34	34	68	915.3
34	60	94	852.1
16	14	30	401.5
16	16	32	401.0

Comparing the composition profile of the tall prefractionator with that of the base system (Fig. 2) indicates less mixing in feed tray while more remixing of middle component is observed. For the numerical comparison of the thermodynamic efficiency, the reflux flow rate to produce the same products from both systems is calculated and listed in Table 2. Increasing the tray number of the prefractionator reduces the reflux flow rate significantly. This explains that the mixing at feed tray has stronger impact on the efficiency than the remixing of the middle component. The explanation is evident when the outcome (Fig. 4) from to the system having 34 trays of a prefractionator and 34 trays of the middle section of a main column is compared with the base system (Fig. 2). The remixing of the intermediate component is nearly same, but the mixing in feed tray of the 34–34 system is less than the base system and the reflux flow rate is lower. Note that the total numbers of trays are same.

When 26 more trays are added to the prefractionator of the 34–34 system, less mixing in feed tray is observed while

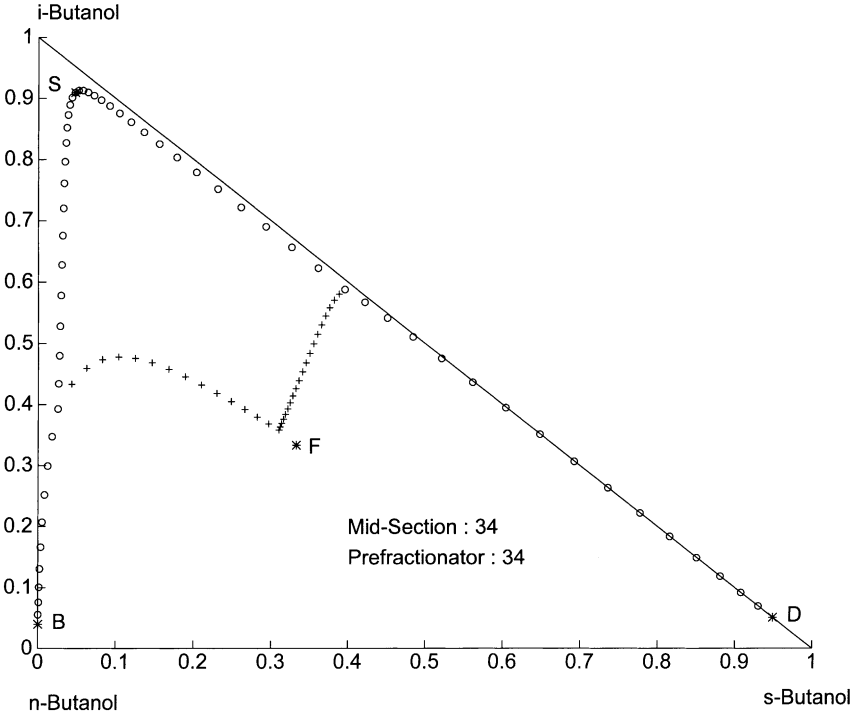

Fig. 4. Liquid composition in a fully thermally coupled distillation system with 34 tray mid-section and 34 tray prefractionator.

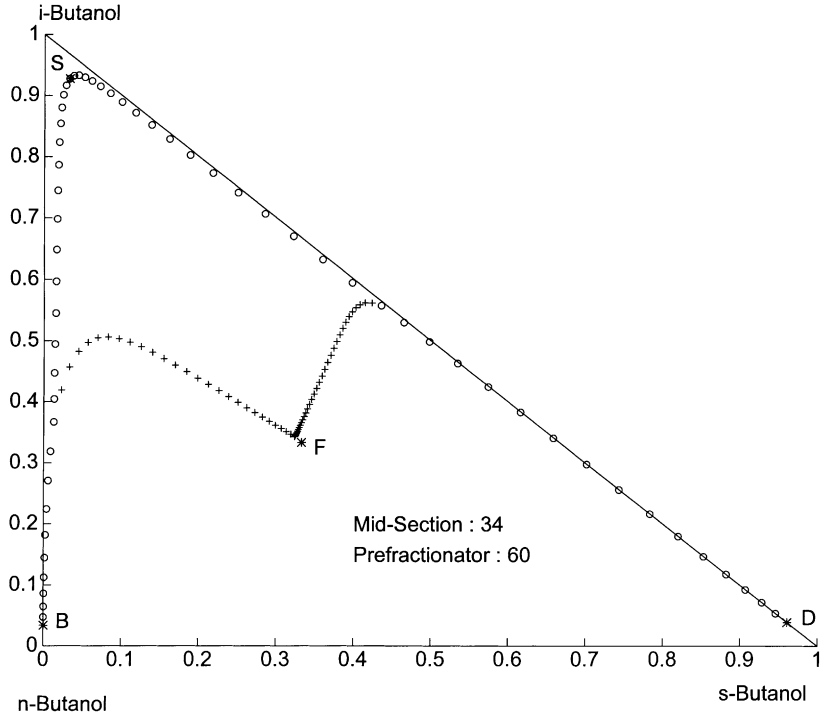

Fig. 5. Liquid composition in a fully thermally coupled distillation system with 34 tray mid-section and 60 tray prefractionator.

more remixing of the intermediate component is shown in Fig. 5. Again, less reflux flow is required to produce same products as listed in Table 2. In this case, the total number of trays is comparable with the 48–48 system, but more reflux flow is necessary although less mixing is resulted. More trays in the middle section of a main column contribute to the reduction.

Since the mixing at the feed tray induces a significant irreversibility in the separation of a ternary mixture, a proper column has to be selected to avoid large mismatch between

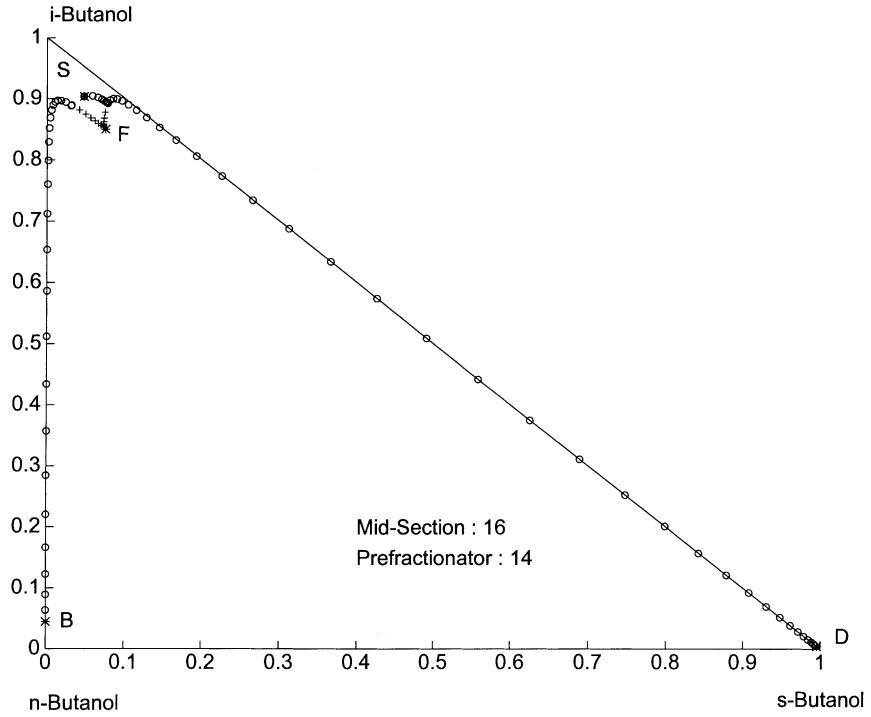

Fig. 6. Liquid composition in a fully thermally coupled distillation system with 16 tray mid-section and 14 tray prefractionator for the feed of high concentration of intermediate component.

the feed composition and the liquid composition at the feed tray. However, a conventional two-column distillation system does not provide a wide variety of feed tray composition in the first column, and therefore the loss of thermodynamic efficiency is inevitable due to the large mismatch in composition. It is because the column must produce at least one high concentration product and the composition profile in the column is shifted to the product. In fully thermally coupled distillation, none of the streams from a prefractionator contain high composition of any of three components and the liquid composition in trays can be adjusted for the feed composition, therefore the composition mismatch in feed tray is much less than that of the conventional system.

When the feed contains high concentration of intermediate component (0.075–0.85–0.075), the mismatch in feed tray is not found as seen in Fig. 6. Moreover, the effect of the increase of tray number of a prefractionator on the mismatch and the reduction of reflux flow are barely noticeable. The liquid composition profile of the taller prefractionator column using the same amount of reflux flow as in Fig. 6 is demonstrated in Fig. 7, and the reflux flow for the equal product with the two different systems is given in Table 2. The commercially operating columns in Japan are processing the feed of very high concentration of intermediate component and the operators from the plant claim that their dividing wall column utilizes less steam than the conventional two-column system by about 40% [22].

8. Multiple solutions

The multiple solutions for the same product composition in fully thermally coupled distillation have been investigated in many studies [2,4,12,23] ever since Chavez et al. [8] published their existence. Because of the multiple steady states, the design of operating condition for a certain product specification includes the search of the optimal reflux flow rate by changing the liquid and vapor split ratios between a main column and a prefractionator. The extra degree of freedom in an FTCDC comparing with a conventional distillation has relation with the existence of the multiple steady-state solutions.

In the relation between liquid split and vapor boil-up [12], there are three regions of liquid split in which no operation is available. At high and low ends of the split ratio, liquid flow rate is less than minimum flow in either a main column or a prefractionator and column operation is not possible there. However, there is a region of no operation in the middle of the split. Because of the middle hole, four split ratios can give same product while the liquid and vapor flow rates are same. In other words, there are four solutions for the same product and operation condition. This is shown in the computation result of Lin et al. [23]. Though there are multiple solutions, the optimum liquid flow obtained from the operational design gives the best solution.

In the design of an FTCDC, the multiple solutions make the conventional design complicated. Without the structural information, an iterative computation using arbitrary

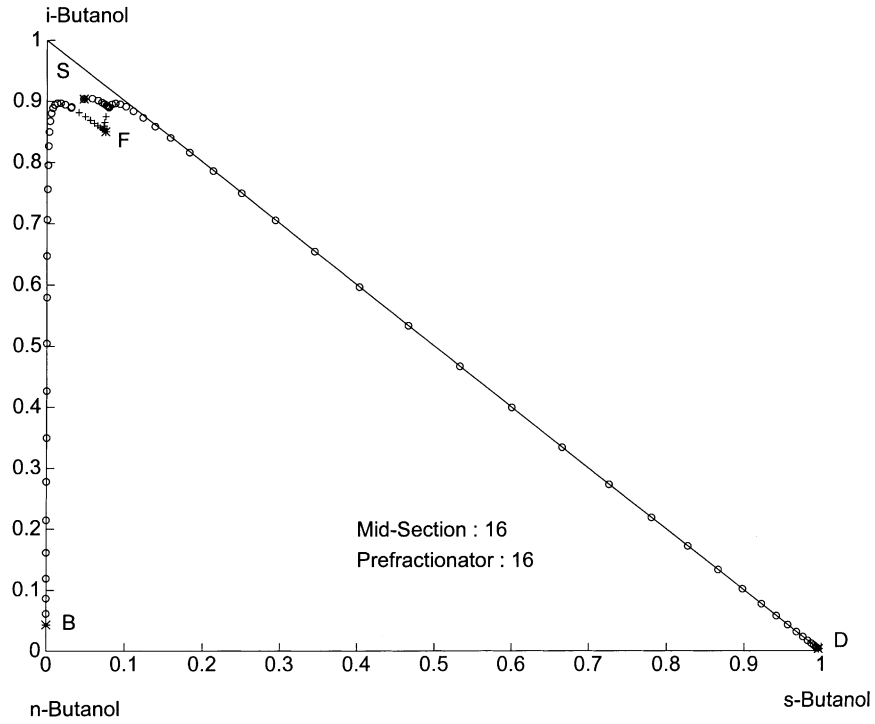

Fig. 7. Liquid composition in a fully thermally coupled distillation system with 16 tray mid-section and 16 tray prefractionator for the feed of high concentration of intermediate component.

structure often leads to the divergence of composition calculation and the multiple solutions make the design more difficult.

9. Petlyuk column versus dividing wall column

For the simplicity of construction, low heat loss and small construction space, a dividing wall column is widely adopted in the commercial applications of an FTCDC [22,24]. In the case, an equal or close number of stages in a prefractionator and the middle section of a main column is necessary. Though the stage number can be adjusted using different tray spacing or packing material, the possible adjustment number is limited. The structure of the dividing wall column has a couple of problems. First, the manipulation of liquid and vapor split is difficult. The adjustment of flow rates of interlinking streams between the prefractionator and the main column is unlikely in the dividing wall column structure. Second, the intentional adjustment of the stage numbers prevents from the optimal design of the system. Moreover, an iterative recalculation to find an adjusted stage number is required from the original number of trays obtained with a standard design procedure, which results in computational burden.

However, the most important point to be considered is that the intentional adjustment leads to the irreversible remixing of intermediate component and reduces the thermodynamic efficiency of the column. In order to avoid the irreversibility of the operation, a separate prefractionator has to be built in spite of the complicated construction.

The advantage of the dividing wall column is its simplicity of construction. However, the manipulation of the distribution of liquid and vapor flow between a prefractionator and a main column is impossible in the column. Also, heat transfer between two contacted sections of the dividing wall column affects design and operation of the column. These disadvantages are not involved in the Petlyuk column.

10. Interlinking streams

In ternary separation, feed has lower concentration of the intermediate component than the side product, and therefore the tray number of a prefractionator is fewer than the mid-section of a main column as shown in Fig. 2. In the case that the tray number in a prefractionator is smaller than the mid-section of a main column, placing the prefractionator in the middle of the mid-section allows the liquid streams of the prefractionator flow by gravitational force. Also, there is less pressure drop in the prefractionator than in the mid-section because the prefractionator has fewer trays. Then vapor will flow from the lower section of a main column to the bottom of the prefractionator and from the top of the prefractionator to the upper section of the main column without an external mechanical work.

When feed has high concentration of the intermediate component, the difference in the tray number between the

prefractionator and the mid-section is small and the interlinking liquid and vapor flows require external work because of the small difference of pressure drops in the prefractionator and the mid-section of the main column. In this case, a modified structure can be utilized. Agrawal and Fidkowski [9] proposed modified structures of the original Petlyuk column by rearranging a section of a main column in order to give easy vapor flow. Also, the dividing wall column structure is favorable for the system of the high concentration of intermediate component in feed, and it is commercially implemented.

11. Operation scheme

The most likely controlled variables in the operation of an FTCDC are the compositions of overhead, bottom and side products. Especially, the concentration of the lightest component in the overhead product, the heaviest component in the bottom product and the intermediate component in a side product are the most convenient set of the controlled variables.

From the operation of a binary distillation column, one can find some guideline for the operation of the Petlyuk column. Most industrial binary columns are operated with one-point control: either the composition of overhead or bottom product [25]. Similarly, the Petlyuk column can be operated using two-point control. Two of the three controlled variables mentioned above are adjusted, where the control problem is much easier than three-point control. However, the two-point control does not give the best regulation of all three products and the most economic operation.

A 3×3 control is suggested by Wolff and Skogestad [12] with the structure of outputs of x_{D1}–x_{B3}–x_{S2} and inputs of *L*–*V*–*S*, and satisfactory control performance is observed except the set-point change of x_{S2}. Symbols of input are shown in Fig. 1. They explain that the problem is from the strong non-linearity from *V* to x_{S2}. For the case that the two components of side product are specified, two 4×4 control schemes, x_{D1}–x_{B3}–x_{S1}–x_{S2} and *L*–*V*–(R_L or R_S)–*S*, are examined. R_L is the ratio of L_2/L and R_S is the fraction of upper side draw of two side product operation. The gain matrices of both four-point controls indicate that x_{S1} is insensitive to paired input to make the control infeasible.

A complete search for the possible 3×3 control schemes is conducted by Mizsey et al. [26] by comparing various controllability indices for multivariable systems. Using the steady-state gains of the schemes, three input sets of *D*/*V*–*S*–*B*, *L*–*S*–*B* and *R*–*S*–*B* are found to be plausible to control the outputs of x_{D1}–x_{S2}–x_{B3}. A regulatory control with changes of feed flow rate and feed composition is applied to examine the control performances of the possible control schemes, and it is found that the input set of *L*–*S*–*B* gives the best control. As indicated in the study, the control scheme may not be valid for other compositions of feed. Also, other control schemes derived by swapping between input variables (cross pairing), e.g. *L*–*S*–*B* and *L*–*B*–*S*, are not investigated.

The suggested *L*–*S*–*B* structure is examined for the case of this study, and the steady-state gain matrix leads to negative diagonal elements in the relative gain array (RGA) [27]. Instead, *D*–*V*–*S* structure is implemented since the structure gives positive elements of the RGA and positive Niederlinski index (NI) [28]. In the selection process of the suggested control structure, open-loop step tests are conducted with possible manipulated variables and an interesting response is yielded. The flow rate of side product affects only the composition of bottom product. Therefore, the flow rate is selected as manipulated variable for bottom product composition in the design of multivariable control scheme. This is not included in the complete search of control scheme for an FTCDC [26]. The array of steady-state gains of x_{D1}–x_{S2}–x_{B3} for the 1% increase of inputs, *D*–*V*–*S*, from their steady-state value is

$$\boldsymbol{G} = \begin{bmatrix} -7.68 & 3.58 & -0.15 \\ -0.85 & 1.82 & -0.88 \\ 5.07 & -0.95 & 5.01 \end{bmatrix} \tag{4}$$

where the values are multiplied by 1000. The diagonal elements are 1.01, 1.09 and 0.87 and the NI is 0.90. This control scheme was suggested by Abdul Mutalib and Smith [4].

12. Column control

The conventional PID control is implemented in the investigation of the performance of the proposed control scheme [4], but an advanced control, the quadratic dynamic matrix control [29] is utilized in order to obtain improved performance. It is widely known that the difficulty of operation of the Petlyuk column has been one of major obstacles in its application. The difficult operation of the column using the conventional control is expected, so the model predictive control is applied. With the sampling time of 30 s, 200 steps are used for the model in each pair of input–output relation and three steps of control horizon.

The controlled variables are compositions of the lightest component in overhead product, middle one in side product and the heaviest one in bottom product, and the manipulated variables are flow rate of overhead product, vapor boil-up rate and flow rate of side product. The split ratios of liquid and vapor between a main column and a prefractionator from the column design are 1.67 and 1.07, respectively. The distribution is manipulated at the design value during the investigation of control performance.

The dynamic matrix of 3×3 multivariable process is yielded from the step response of the controlled variables, and predicted error and manipulated variable are related as

$$\boldsymbol{e} = \boldsymbol{A}\boldsymbol{u} \tag{5}$$

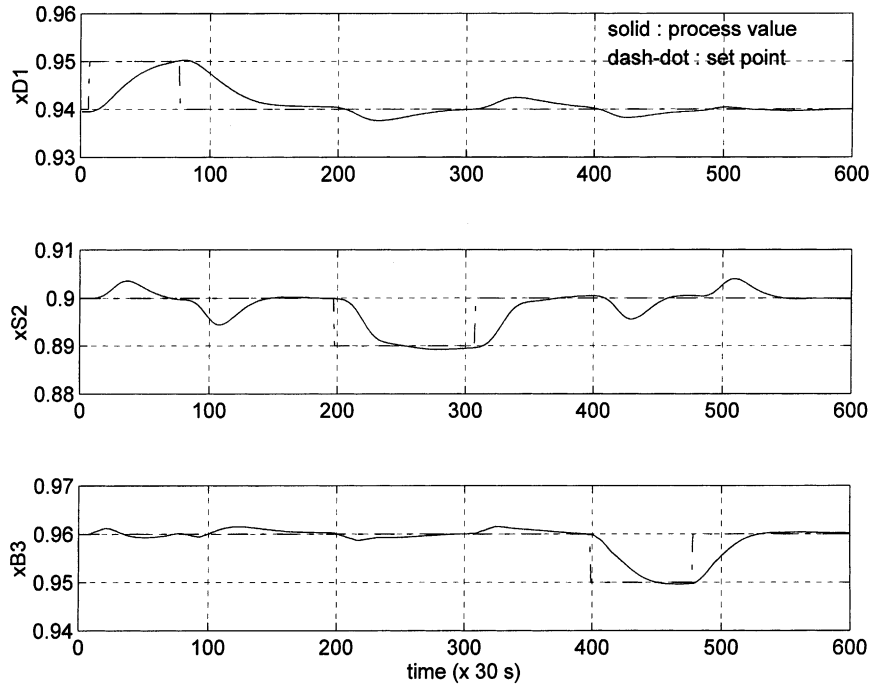

Fig. 8. Set-point tracking performance of a 3×3 control scheme using the quadratic dynamic matrix control.

where $\boldsymbol{A}$ is the dynamic matrix, $\boldsymbol{u}$ the manipulated variable and $\boldsymbol{e}$ is the error which is computed from Eq. (6):

$$\boldsymbol{e} = \boldsymbol{y}_{\mathrm{S}} - \boldsymbol{y}^{*} - \boldsymbol{d} \tag{6}$$

where $\boldsymbol{y}_{\mathrm{S}}$ is set-point, $\boldsymbol{y}^{*}$ the predicted output and $\boldsymbol{d}$ is the unmeasured disturbance. The control objective is formulated as a quadratic minimization problem:

$$\min \boldsymbol{J} = \tfrac{1}{2}\boldsymbol{u}^{\mathrm{T}}\boldsymbol{H}\boldsymbol{u} - \boldsymbol{g}\boldsymbol{u} \tag{7}$$

s.t.

$$\boldsymbol{C}\boldsymbol{u} = \boldsymbol{b}$$

$$\boldsymbol{u}_{\min} \leq \boldsymbol{u} \leq \boldsymbol{u}_{\max}$$

where

$$\boldsymbol{H} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{\Gamma}^{\mathrm{T}}\boldsymbol{\Gamma}\boldsymbol{A} + \boldsymbol{\Lambda}^{\mathrm{T}}\boldsymbol{\Lambda}$$

and

$$\boldsymbol{g} = \boldsymbol{A}^{\mathrm{T}}\boldsymbol{\Gamma}^{\mathrm{T}}\boldsymbol{\Gamma}\boldsymbol{e}$$

where $\boldsymbol{\Gamma}$ and $\boldsymbol{\Lambda}$ are control tuning parameters. The first constraint is formulated from the limit of total variation of the manipulated variable, and the second is of a single-step variation. This problem is solved using the IMSL, a commercial software, and the solution $\boldsymbol{u}$ is implemented as a manipulated variable. The constraints are composed of the limit of manipulated variable. The upper limit of the variable is +5% from its steady-state value and lower limit is −5%. A single-step variation of the variable is set to 0.1% of the steady-state value. The diagonal elements of control tuning parameters of $\boldsymbol{\Gamma}$ and $\boldsymbol{\Lambda}$ are all given with one.

The set-point changes of three components are imposed separately and the response is shown in Fig. 8. In the top of the figure, the composition of overhead product varies as the set-point is raised and returned to the initial value while the composition of side product is affected by the change and shows some deviation from its set-point. However, the composition of bottom product fluctuates very little. When the set-point change of side product composition is applied in the same manner, nearly similar deviation in overhead and bottom products is observed, but the magnitude of the deviation is much less than the previous case. In the change of bottom product composition, the deviation of side product composition is nearly same as the outcome of the change of overhead product composition and the deviation of overhead product composition is not significant. The control performance of the set-point tracking in all three products is satisfactory, since no significant deviation from the set-point is developed though the response is slow. Though different system is studied in Abdul Mutalib and Smith [4], more step change of set-point is applied in this study and better control performance is yielded.

A regulatory performance is examined by changing feed flow rate and feed composition as given in Fig. 9. In the bottom figure, the first 200 steps denote the variation of feed flow rate and should be read from the scale on the left ordinate. The rest of the 600 steps are of the composition of lightest component in feed and use the scale of the right ordinate. The initial feed composition is equimolar mixture of *s*-butanol–*i*-butanol–*n*-butanol and the varied composition is 0.32–0.34–0.34. The effect of a 2% change of feed flow rate is not significant, but the impact of the change of feed

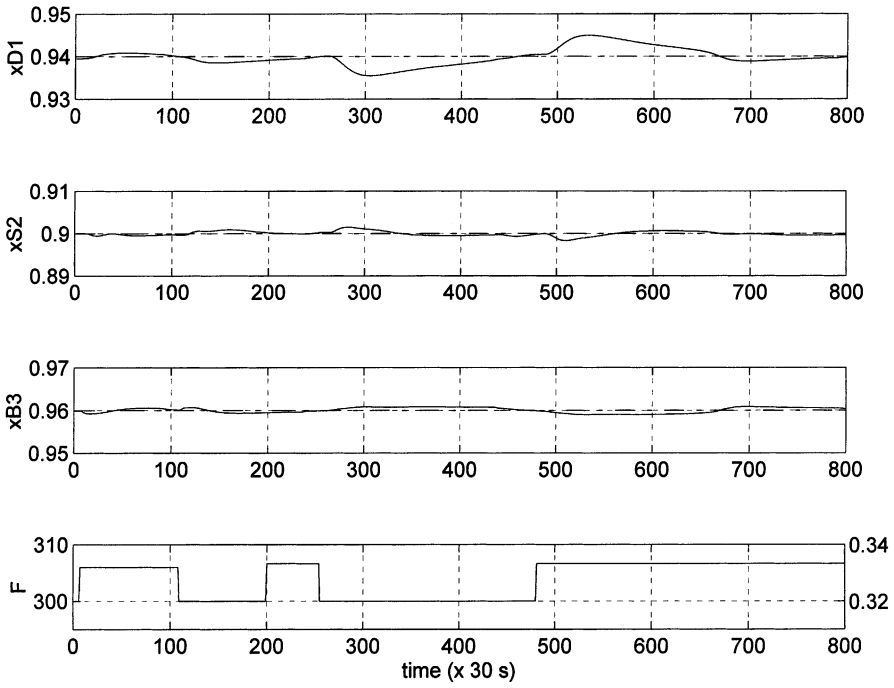

Fig. 9. Regulatory performance of a 3 × 3 control scheme using the quadratic dynamic matrix control.

composition is much greater. Since the lightest component has the largest change in composition, its deviation is the highest among three components.

13. Conclusion

A structural design procedure for fully thermally coupled distillation columns is exercised to an example system having different compositions of feed. The structural information from the design eliminates tedious iteration encountered in the design using conventional procedures. From the result of the design for the example system and the comparison of calculated liquid composition with a commercial design tool, it is proved that the proposed procedure is useful.

In addition, other design related subjects, such as thermodynamic efficiency, dividing wall structure and the arrangement of interlinking streams, are investigated using the information of the structural design and possible improvements concerning the subjects are suggested. Mixing in feed tray reduces the thermodynamic efficiency more than the remixing of intermediate component. A separate prefractionator system is better than the dividing wall structure unless the concentrations of intermediate component in feed and side product are close.

For the column operation, a 3 × 3 control scheme is adopted and its performance of set-point tracking and regulation with a model predictive control is examined to result in satisfactory outcome.

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