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Design of a Fully Thermally Coupled Distillation Column Based on Dynamic Simulations

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Abstract−A dynamic simulation of a fully thermally coupled distillation column is conducted for the design of a possible operation scheme, and its performance is examined with an example process of butanol isomer ternary system. The outcome of the dynamic simulation indicates that the column can be operated by using a 3×3 control structure. The structure consists of three controlled variables of the compositions of overhead, bottom and side products and three manipulated variables of the flow rates of reflux and steam and liquid split ratio between a main column and a prefractionator.

Key words: Process Design, Distillation Column, Thermally Coupled Column, Dynamic Simulation, Petlyuk Column

INTRODUCTION

Though the fully thermally coupled (Petlyuk) distillation [Petlyuk et al., 1965] was introduced a half century ago, it was not commercially implemented until recently owing to the difficulty of its design and operation. Its principle is that two distillation columns separating three components from a ternary mixture are converted into a single column and a prefractionator having neither reboiler nor condenser. That means two columns are operated with one reboiler and one condenser, and therefore heat requirement is much less than that of a conventional two column system. A schematic diagram of the Petlyuk column is shown in Fig. 1.

In the design of the fully thermally coupled distillation system, a simplified short-cut method [Triantafyllou and Smith, 1992] has been utilized for the simplicity of the design. However, its design accuracy is not sufficient enough to be employed as an initial design for the coupled distillation system.

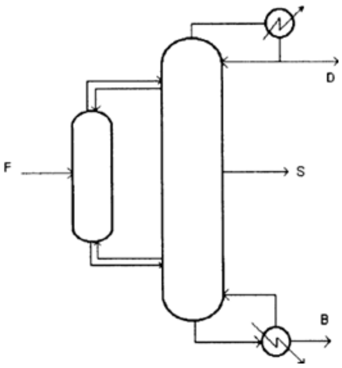

Fig. 1. Schematic diagram of a fully thermally coupled distillation column.

The operational scheme of a fully thermally coupled distillation was examined by Wolff and Skogestad [1995], and it is 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 as a variation of the Petlyuk column, the sensitivity of liquid and vapor splits between prefractionator and main column is explored for the control of impurity in side product [Abdul Mutalib and Smith, 1998]. Yet they conclude that the liquid and the vapor splits should be kept constant at the highest product specification since the composition of the side product is insensitive to the variation of the splits.

In this study, a rigorous design procedure of a fully thermally coupled distillation column is explained to find initial operation information used in the dynamic simulation. Then the procedure of the dynamic simulation of the fully thermally coupled distillation column is proposed, and the simulation is applied to find a possible operation scheme of the column. The whole procedure is applied to an example system of butanol isomer ternary mixture.

COLUMN DESIGN

In order to generate the initial set of operation variables to be implemented in the dynamic simulation, a rigorous design of a fully thermally coupled distillation column has to be conducted. In this section, the design procedure is briefly explained.

In the design of a fully thermally coupled distillation column, the minimum number of trays is computed first instead of the minimum flow because an extra design variable, the location of inter-linking stages, is necessary unlike in the design of conventional distillation columns. After the minimum numbers of trays of a prefractionator and a main column and the inter-linking stages are obtained, the numbers are proportionally increased for a practical column with a given reflux flow rate. The number of trays in a prac-

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tical distillation column of this study is taken as twice the minimum number.

The minimum reflux flow rates for a prefractionator and a main column [Fidkowski and Krolikowski, 1986] are implemented to calculate the liquid split ratio. When a trial liquid flow and vapor boilup rates are given, the initial flow rates are readily found by using the equimolal overflow assumption. Then, the tray liquid composition is evaluated from a steady state material balance. The vapor composition is replaced with a liquid composition and an equilibrium constant obtained with the UNIQUAC equation. The vapor flow rate is calculated from an energy balance, and the liquid flow rate is from a total material balance in a tray. The material balances are converted to a matrix form, and the liquid composition is yielded from matrix inversion. This procedure is iteratively continued until the variation of tray temperature is less than a given limit, say 0.0001 times total number of trays. In order to improve the convergence of the iterative computation, a relaxation factor is added to the renewal of liquid composition.

The compositions of overhead, bottom and side products obtained from the liquid compositions are compared with the specification. If the specification is not satisfied, different reflux flow and vapor boilup rates are tried until on-specification products are yielded. The liquid split ratio needs to be checked if the ratio gives the optimum reflux flow rate, since the computed minimum flow is larger than the true minimum flow in some cases [King, 1971].

DYNAMIC SIMULATION

The difference between the rigorous design of the previous section and the dynamic simulation of a fully thermally coupled distillation column is the way of composition computation. In the design, the column operation is assumed to be at the steady state; therefore, a tray liquid composition is directly yielded from the steady state material balance. In the dynamic simulation, however, the composition is found from the unsteady state component material balance of liquid holdup in trays. The initial information of operation, such as liquid and vapor flow rates, liquid composition and temperature, is computed from the rigorous simulation and fed to the dynamic simulation. In the rigorous model for the dynamic simulation, ideal tray efficiency is assumed. Also, vapor holdup is ignored for the holdup, which is much less than liquid holdup. The detailed procedure of the simulation is summarized in Table 1.

Table 1. Procedures of dynamic simulation

Step	Procedure
1	read initial liquid and vapor flow rates, composition and temperature
2	find initial tray holdup using Francis weir equation
3	compute vapor composition using the UNIQUAC correlation
4	compute enthalpy of liquid and vapor in each tray
5	obtain vapor flow rates from energy balances
6	find new liquid composition from material balance of component liquid holdup
7	calculate liquid flow rates from tray liquid holdup
8	accept new operating condition, if any
9	go to step 3 for next time step

From the initial liquid flow rate, the liquid holdup in trays is computed by using the Francis weir equation [Luyben, 1990]. An exact tray holdup is required, otherwise an erroneous liquid flow rate is yielded from the holdup and the iterative computation does not converge to a solution.

At the liquid composition, the vapor composition and tray temperature are calculated by using the UNIQUAC equilibrium relation. Then the enthalpies of liquid and vapor are evaluated to formulate energy balances at the trays. The vapor flow rate is obtained from the energy balance of the nth tray.

$$M_n = (h_{n+1}L_{n+1} + H_{n-1}V_{n-1} - h_nL_n)/H_n \tag{1}$$

The component material balance is

$$M_n\frac{dx_{n,i}}{dt} = L_{n+1}x_{n+1,i} + V_{n-1}y_{n-1,i} - L_nx_{n,i} - V_ny_{n,i} \tag{2}$$

and the variation of tray holdup of the ith component is computed from the equation. The variation gives the new liquid composition. Similarly, the change of total tray holdup is also yielded as

$$\frac{dM_n}{dt} = L_{n+1} + V_{n-1} - L_n - V_n \tag{3}$$

and the new liquid flow rate is given from the holdup and the Francis weir equation.

After the new set of liquid composition, liquid and vapor flow rates are evaluated, the whole procedure is repeated for the next time step. The simulation time step is set to one third of a second considering the tray time constant, about 10 seconds, found from the average liquid flow rate and the average tray holdup.

RESULTS AND DISCUSSION

A rigorous design procedure is implemented on a ternary system of s-butanol-i-butanol-n-butanol mixture for the equimolar feed. From the design, the total reflux flow rate is found to be 961 mol/h and the liquid split ratio of a prefractionator to a main column is 1 : 1.89. In this operating condition, the variation of tray liquid composition for the column is shown in Fig. 2. When the actu-

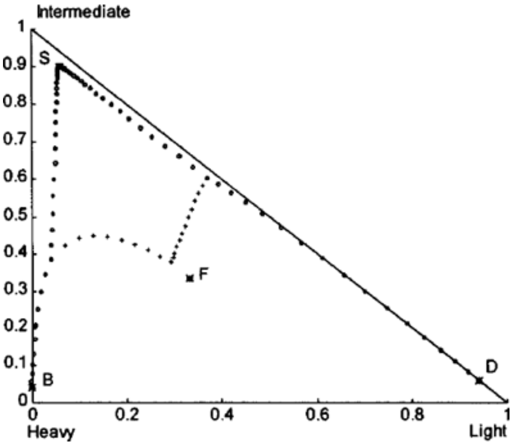

Fig. 2. Liquid composition in a fully thermally coupled distillation column.

al reflux flow rate is compared with the minimum reflux flow rate (694 mol/h), it is 1.4, which is within the range of common practice. Therefore, the tray number taken in this design, twice of the minimum number, is reasonable. The steady state operation variables, such as liquid and vapor flow rates, are provided to the dynamic simulation as an initial condition.

In order to find a possible control structure of the column, some step responses of three product specifications for various manipulated variables are examined. The three specifications are the composition of the lightest component in the overhead product, the intermediate component in a side product and the lightest component in the bottom product. The flow rates of reflux and steam are obvious selections for the manipulated variable and the liquid flow rate in a prefractionator is chosen as the third manipulated variable. Wolff and Skogestad [1995] employed the product flow rate of the side product as a manipulated variable, but its response is not so favorable as the prefractionator liquid flow. Because the liquid flow of a prefractionator comes from a main column, the flow rate gives directly the liquid split ratio between the prefractionator and the main column.

In Fig. 3, the responses are demonstrated for the changes of ±1% and ±2% of reflux flow. Note that the scale of compositions is same in all three products. The largest change among the compositions of three products with the reflux flow is found from the overhead product; therefore, the reflux flow is a likely manipulated variable and can be employed to control the composition of the overhead product. The responses for the steam flow with the same amount of variation as in the reflux flow are given in Fig. 4. In this case, the outcome is similar to the previous figure. Considering bottom product is obtained from a reboiler and the steam is provided to the reboiler, a possible manipulated variable for the control of bottom product composition is the steam flow.

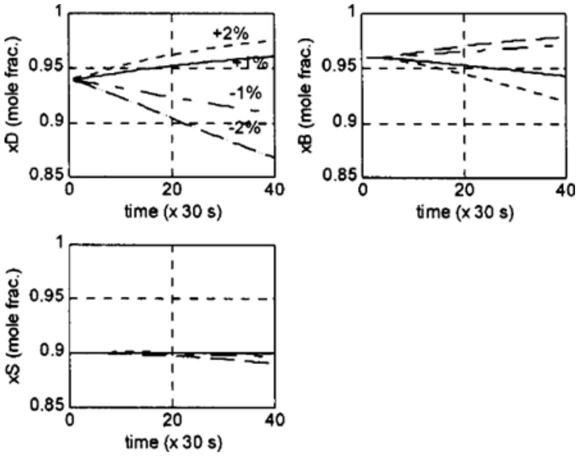

Fig. 3. Step responses of reflux flow rate changes.

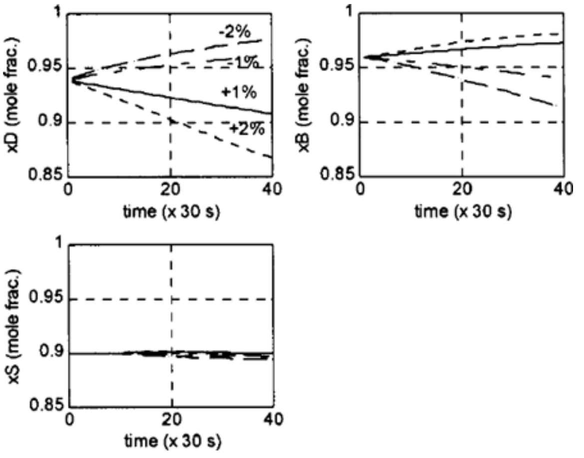

Fig. 4. Step responses of steam flow rate changes.

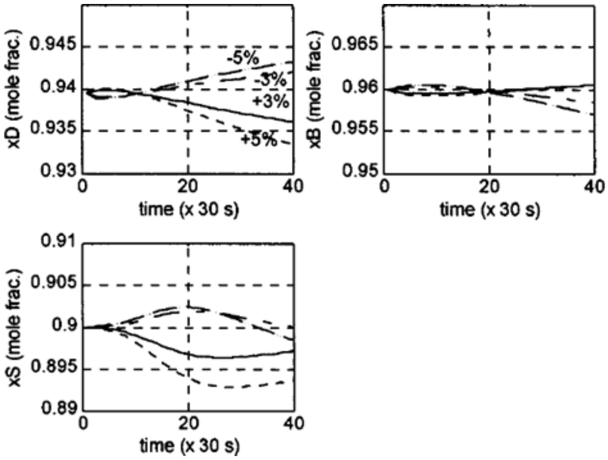

Fig. 5. Step responses of prefractionator liquid flow rate changes.

However, the results for the prefractionator liquid flow are quite different from the previous cases as described in Fig. 5. Note that the composition scale is much smaller than the other two and more changes of the liquid flow are applied. The responses show high nonlinearity, and it is expected that the control of side product composition is very difficult. There are other options to control the composition, such as the flow rate of side product and reflux to the one tray above the tray drawing side product, but the steady state gain is much less than that of the prefractionator liquid flow. Therefore, the only available manipulated variable for the control of side product composition is the flow.

CONCLUSION

A rigorous design procedure for a fully thermally coupled distillation column is applied to find the initial information of operation variables, which is necessary for the dynamic simulation of an example ternary system of s-butanol-i-butanol-n-butanol mixture.

Using the initial values of liquid and vapor flow rates, temperature and liquid composition obtained from the design, a dynamic simulation is conducted to yield step responses for a suggested control structure. Even though the control of the composition of side product is expected to be somewhat difficult from the result of the dynamic simulation, a 3×3 structure looks feasible to operate a fully thermally coupled distillation column.

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NOMENCLATURE

B : bottom product
D : overhead product
H : vapor enthalpy
h : liquid enthalpy
L : liquid flow rate [mol/hr]
M : tray liquid holdup [mol]
S : side product
t : time [hr]
V : vapor flow rate [mol/hr]
x : liquid composition [mole fraction]
y : vapor composition [mole fraction]

Subscripts

B : the heaviest component in bottom product
D : the lightest component in overhead product
i : component i
n : tray number
S : intermediate component in side product

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