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Controllability of separate heat pump distillation for separating isopropanol-chlorobenzene mixture

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Abstract−The isopropanol-chlorobenzene mixture is separated via separate heat pump distillation (SHPD) to achieve significant energy savings. Rigorous steady state and dynamic characteristics for this SHPD process are simulated using Aspen Plus and Aspen Plus Dynamics. Optimized operation conditions including vapor flow rate to compressor are developed on the condition of minimum total annual cost. Two control strategies are proposed to solve feed disturbance issues and the improved structure with Q_{Re}/F (lower column reboiler duty/feed flow rate) ratio scheme can maintain the two product purities requirement with smaller transient deviation and shorter settling time.

Keywords: Dynamic Control, Separate Heat Pump Distillation, Aspen Plus, Isopropanol, Chlorobenzene

INTRODUCTION

Distillation is the most widely used method by far for separating liquid mixtures despite its high energy-consumption. Reports have shown that about 40-60% energy is used in separation unit in the chemical and petrochemical industries [1,2]. The continuous soaring of energy costs, the improving international environmental regulations and the increasing public concern make it inevitable for many to look for ways to reduce energy consumption.

The exploration to improve efficiency and reduce environmental pollution associated with distillation processes is gaining considerable attention. Many energy-saving technologies, including heat pump distillation [3], thermally coupled distillation [4,5], inter-reboiler and inter-condenser distillation [6] and multi-effect distillation [7], have been developed to promote the development of distillation technology. In addition, specific distillation processes, including pressure-swing distillation [8-10], extractive distillation [11] and dividing-wall columns [12], concern on energy-saving very much.

Many experimental researches have proved that heat pump-assisted distillation technology is a promising and successful heat integration technology to reduce energy consumption and decrease negative effects on the environment compared with conventional distillation. Conventional direct vapor recompression heat pump distillation is usually applied to separate close-boiling mixtures. Design, modeling and optimization of the conventional heat pump distillation have been studied by many researchers [13-19]. However, for wide-boiling mixture, using the compressed top steam as the direct heat source of the bottom would result in too much energy consumption of the compressor, which leads to an increase in the equipment investment cost and operating cost [20]. Therefore, a more energy efficient method is needed.

For some binary mixtures with large relative volatility in the low concentration range and small relative volatility in the high concentration range, the conventional distillation column can be divided into two columns with an upper and lower column. The upper column can adopt the conventional heat pump-assisted distillation technology because of the small temperature difference between its top and bottom, whereas the lower column is equivalent to a traditional distillation column. The above process, called separate heat pump distillation (SHPD), usually saves energy significantly. Zhu and Feng [21] investigated the economic feasibility and operability of the SHPD process to separate ethanol and water system. The SHPD process and three other distillation schemes, namely, conventional single-column distillation, multi-effect distillation, conventional heat-pump distillation, were proposed to separate methanol-chlorobenzene by Gao et al. [22] and results show that the SHPD process has an obvious energy-saving effect compared with the other distillation processes.

The performance of dynamic control is another important factor for a distillation process. Control of the conventional heat pump distillation process and other heat-integrated distillation processes has been studied recently [23-35]. Karami et al. [31] studied controllability of two processes of conventional heat pump-assisted distillation columns. Yu et al. [34] presented various control structures for pressure-swing distillation with full heat integration to separate the mixture of methylal and methanol. Zhang et al. [35] proposed three control structures for the separation of isopropyl and ethyl acetate by using an extractive dividing-wall column. However, control of the SHPD process is much more difficult than conventional heat pump distillation process and other heat-integrated distillation processes because of its complex inner structures and strong interactions among control loops in the SHPD process, and there is no report about the control of SHPD process.

We present here an SHPD process for the separation of isopropanol/chlorobenzene. An optimized design for this SHPD process is demonstrated using total annual costs (TAC) as an objective function. For the optimized SHPD process, control structures were ex-

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plored for the first time and their dynamic characteristics were evaluated.

STEADY STATE DESIGN

1. SHPD Process for the Separation of Isopropanol-chlorobenzene Mixture

The T-x(y) phase diagram at atmospheric pressure for the isopropanol-chlorobenzene system is shown in Fig. 1. The isopropanol and chlorobenzene mixture has a high relative volatility in the low composition range, and low relative volatility in the high composition range. It is feasible to design a distillation process by dividing a distillation column into two parts to separate the mixture. The upper column is installed with a heat pump and the lower column works as a conventional distillation column. Hence, an SHPD process is formed and its economics is calculated.

Fig. 2 shows the schematic diagram of the SHPD process. The upper column has similar characteristics as the conventional direct

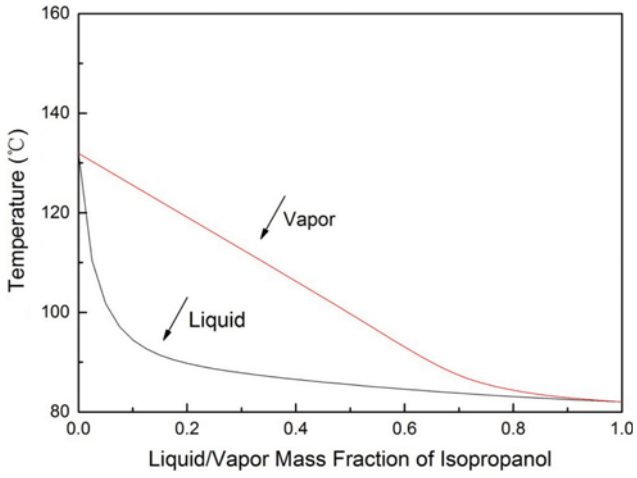

Fig. 1. T-x(y) phase equilibrium diagram for the isopropanol-chlorobenzene system.

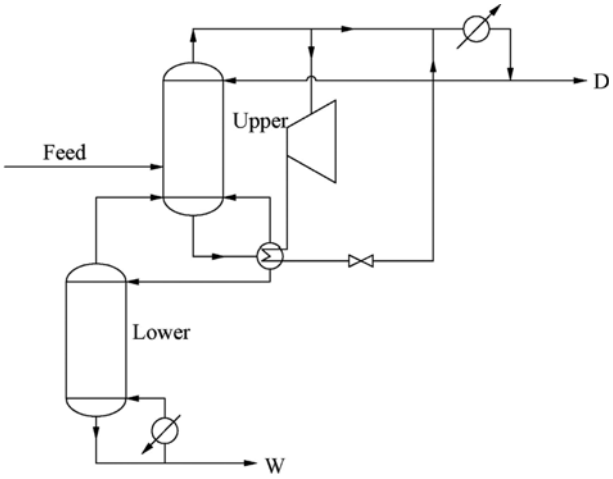

Fig. 2. Schematic diagram of the separate heat pump distillation process.

mechanical vapor recompression heat pump distillation, except an extra vapor phase feed inlet near the bottom. From the top of the upper column, part of the overhead vapor is recompressed by a compressor for heating the bottom. The rest of the overhead vapor is condensed by using an auxiliary condenser. Part of the mixture condensate in the drum is withdrawn as the product and the rest is returned into the upper column as the reflux. The lower column works a similar function as the stripper section of the conventional distillation column. The feed liquid is fed to lower column from the bottom liquid of the upper column and the out-coming vapor from lower column enters at the bottom of upper column. In the high composition range (x=0.85-1 (mass fraction)), the temperature lines of liquid (x) and vapor (y) are close, as the relative volatility of the isopropanol and chlorobenzene mixture is near 1. In the low composition range (x=0-0.85), however, the isopropanol and chlorobenzene mixture has a large relative volatility. Hence, the reflux ratio of the lower column is significantly smaller than that of the upper column.

2. Process Design

The fresh feed is a liquid mixture containing 30 wt% isopropanol and 70 wt% chlorobenzene at a mass flow rate of 5,000 kg/h. The operation of the column is under atmospheric pressure. The commercial software of Aspen Plus and Aspen Dynamics was employed for the rigorous steady state and dynamic simulations in this study. The vapor-liquid equilibrium calculated data of isopropanol and chlorobenzene using the UNIQUAC model in the Aspen Plus fit well with the experimental data [36]. Hence, the UNIQUAC property model was chosen as the thermodynamic model. The required products purities for the isopropanol and chlorobenzene are 99.8 wt% or above.

The economics for conventional single-column distillation process in the same conditions was compared with the SHPD process. The simulation of the compressor, distillation columns and heat exchangers were employed by using the Compr, RadFrac and Heatx blocks, respectively. The isentropic efficiency of compressor was 0.72. The temperature difference between the bottom of the upper column and the compressor outlet was limited to 10 °C.

3. Optimization Variable for SHPD Process

It cannot be considered that SHPD is simply dividing a column into two columns. The split point where the column is divided has a great influence on the capital investment and the operating costs of this system. The split point composition is a key variable for SHPD process and it was taken as the optimization variable by Gao et al. [22]. It is difficult to control the split point composition when the feed disturbances are introduced during the dynamic simulation because the split point concentration is a state variable. The vapor flow rate to the compressor is used as an optimization variable to minimize TAC. The vapor flow rate to the compressor is regulated by changing top steam split ratio of the steam splitter. The effect of the vapor flow rate to compressor on concentration of split point, the equilibrium stages, the compressor power, the loads of the auxiliary condenser and the lower column reboiler, and the TAC are given in Table 1.

For a given separation, the greater the vapor flow rate to the compressor, the smaller is the concentration at the split point, and hence, the separating duty for the lower column would decrease, resulting

Table 1. Simulation results for different vapor flow rate to compressor

		Upper column			Lower column	
M_{D3}	$X_{isopropanol}$	D (m)	Q_C (kW)	W_m (kW)	D (m)	Q_{RE} (kW)
3260	0.28	0.7360	476.39	96.22	0.5166	403.75
3120	0.29	0.7359	497.27	77.98	0.5413	442.72
3000	0.30	0.7348	514.22	72.59	0.5546	465.01
2860	0.31	0.7340	533.05	70.49	0.5671	485.94
2750	0.32	0.7333	548.06	63.52	0.5798	507.81
2565	0.33	0.7333	571.38	61.75	0.5940	532.76
2340	0.34	0.7333	583.80	48.91	0.6082	557.65
2250	0.35	0.7333	606.21	46.04	0.6221	583.17
2100	0.36	0.7333	630.11	42.97	0.6362	610.04
1940	0.37	0.7333	656.01	38.94	0.6526	639.92
1780	0.38	0.7332	681.99	35.67	0.6667	668.95

M_{D3}, vapor flow rate to compressor; $X_{isopropanol}$, slit-point concentration; D, diameter of column; Q_C, load of condenser; W_m, input power of compressor; Q_{RE}, load of lower reboiler

in a decrease in the capital investment and operating costs for the upper column. Moreover, the greater the vapor flow rate to compressor, the lesser to the auxiliary condenser; thus, a smaller auxiliary condenser area and the lesser cooling water flow is required. However, the split point composition and the separating duty for the upper column would increase with the increase of vapor flow rate to the compressor, making an increase in the capital investment and operating costs for the upper column and compressor. Accordingly, the split point composition and the vapor flow rate to the compressor are inherently interdependent, but the latter variable can be

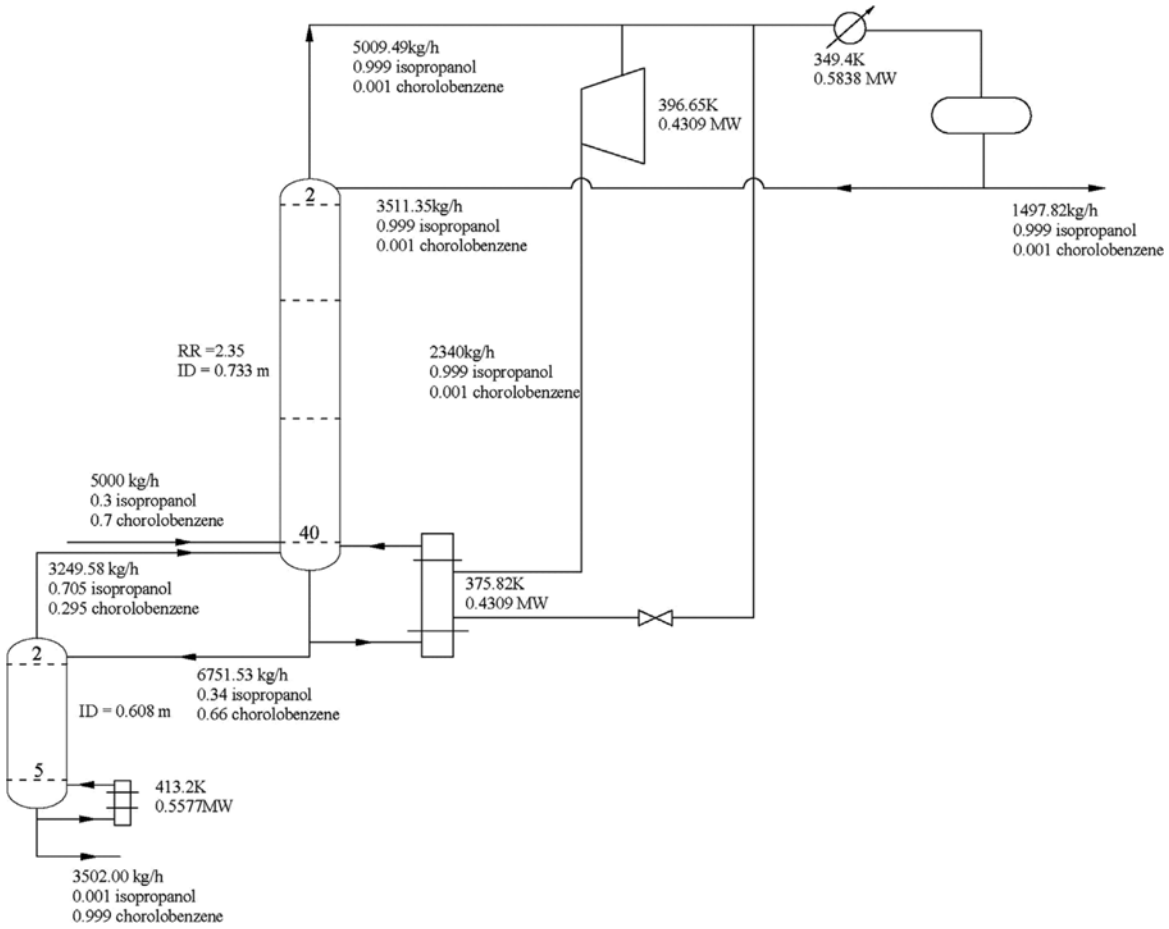

Fig. 3. Flowsheet for the optimized SHPD process.

easily controlled by an overhead vapor splitter. Therefore, the optimal design of the SHPD process uses the vapor flow rate to the compressor as an optimization variable.

TAC is used as the objective function to screen process candidates, which includes annualized operating costs and capital costs. The total operating costs (TOC) include the steam for the reboiler of the lower column (C_S), the cooling water for the auxiliary condenser (C_{CW}), and the electricity for the compressor (C_{Ele}). The capital costs include the two distillation column shells, the compressor, condenser, reboiler, and a payback period of three years is assumed. Other items such as pumps, reflux drums, pipes, and valves are usually not considered because of their much lower costs than the costs of the compressor, heat exchangers, and column shells. The costs of utilities and equipment are taken with formulas as follows:

The annual steam cost is

$$C_S = C_0 \times Q_R \times 8000$$

Note that the steam cost (C_0) is LP steam (433 K)=$7.72 per GJ, MP steam (457 K)=$8.22per GJ, HP steam (527 K)=$9.88 per GJ [37].

The annual cooling water cost is

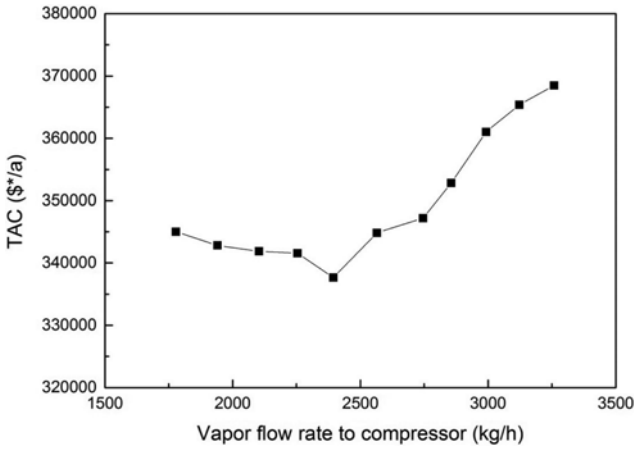

Fig. 4. Simulated relationship between the TAC and the vapor flow rate to compressor.

$$C_{CW} = C_w \times \left(\frac{Q_C}{\Delta T_w \times C_p \times 1000} \right) \times 8000 \times 3600$$

where C_w is the price of cooling water (0.03$/1,000 kg), ΔT_w is

Table 2. Comparison of results for different distillation processes

Distillation process	Q_{RE} (kW)	Q_c (kW)	W_m (kW)	Total capital cost ($\$10^4$/year)	Annual operating cost ($\$10^4$/year)	TAC ($\$10^4$/year)	Saved TAC ($\$10^4$/year)
SHPD	583.80	557.65	48.91	52.13	16.39	33.77	17.44
Conventional single-column distillation	1058.19	1016.57	-	40.02	37.87	51.21	-

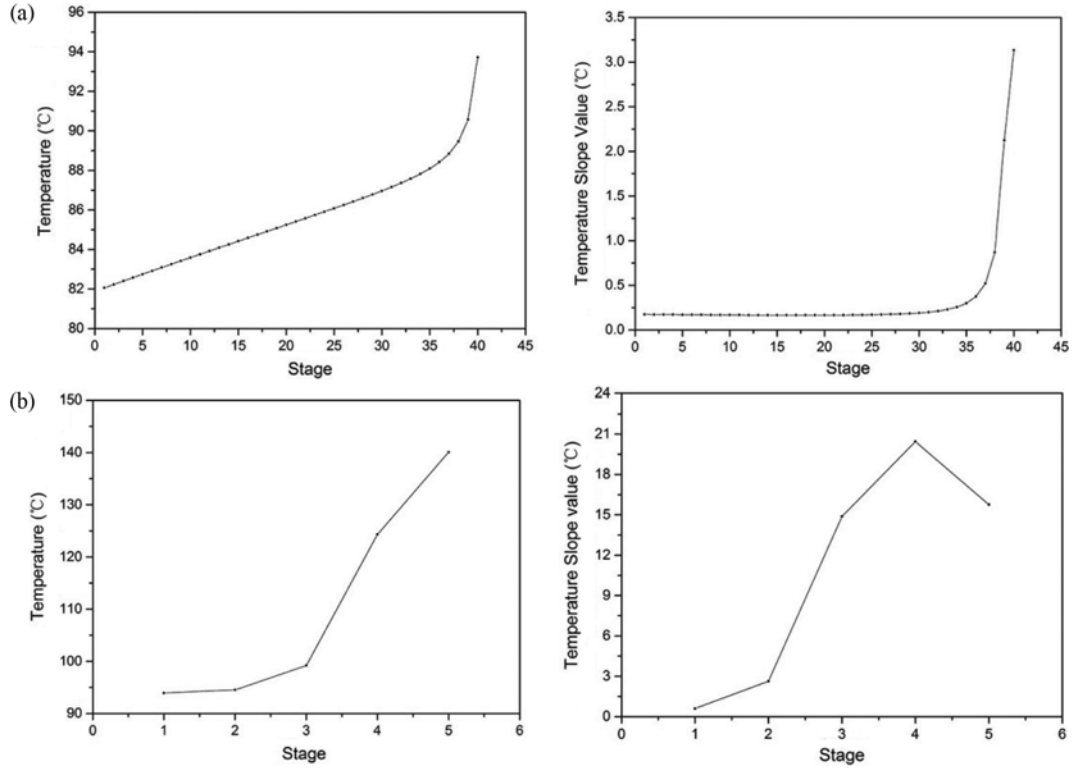

Fig. 5. (a) Temperature profile and temperature slope value plots of the upper column. (b) Temperature profile and temperature slope value plots of the lower column.

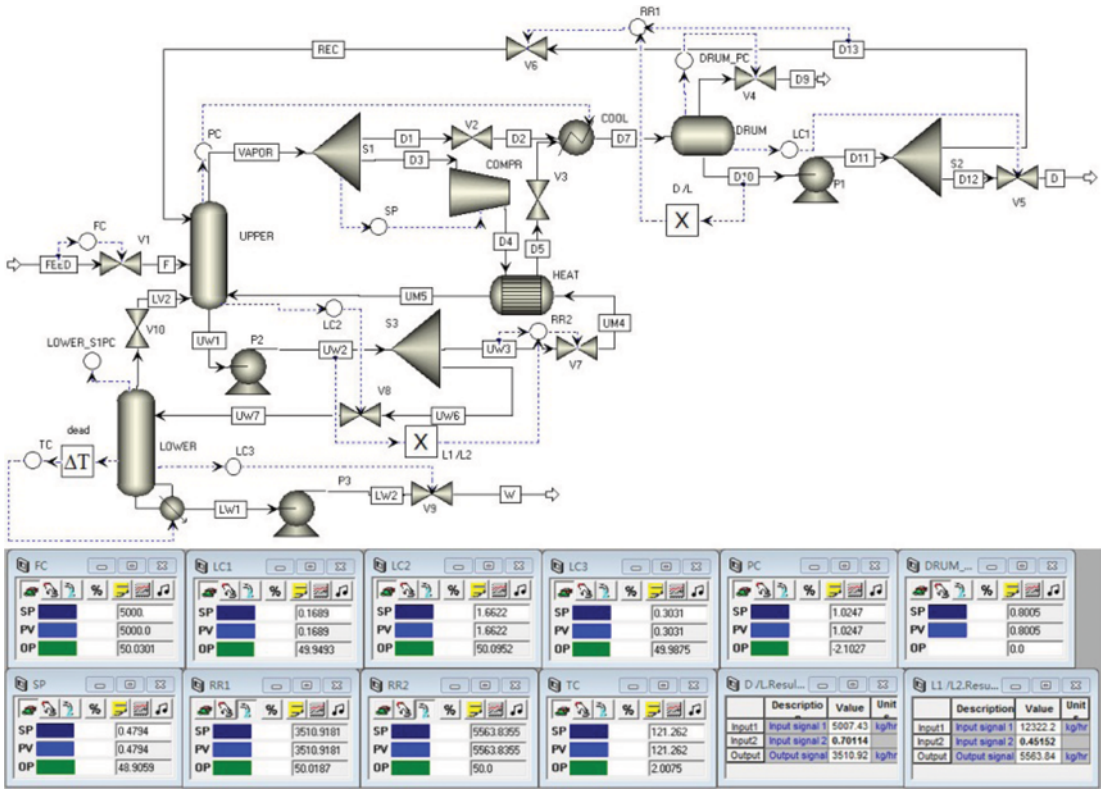

Fig. 6. Basic control structure.

the differential temperature (design with 10 K), and C_p is the specific heat of water.

The electricity cost is

$$C_{Ele}=W_{comp}\times C_e\times 8000$$

W_{comp} is the power of the compressor; C_e=0.09386$/(kW·h).

Hence, the total operating cost is

$$TOC=C_S+C_{CW}+C_{Ele}$$

The column vessel cost is

$$C_{CV}=\left(\frac{M\ \&\ S}{280}\right)\times 5485.17\times D^{1.066}\times H^{0.802}$$

where D is the column diameter (m) and H is the column height (m).

The heat exchanger cost is

$$C_{HE}=\left(\frac{M\ \&\ S}{280}\right)\times 3490.00\times A^{0.65}$$

Note that A is the heat transfer area (m^2). The heat transfer coefficients of the condenser and reboiler are 0.568 and 0.852 kW/($K\cdot m^2$), respectively [38].

And, the compressor cost is

$$C_{Comp}=\left(\frac{M\ \&\ S}{280}\right)\times 1609.42\times (bhp)^{0.82}$$

The bhp=hp/0.73 and the hp is the work of the compressor.

The total capital cost (TCC) is

$$TCC=C_{CV}+C_{HE}+C_{Comp}$$

Hence, the TAC is

TAC=(TCC/payback period)+TOC.

A steady state flowsheet of the SHPD process with detailed steam information, equipment sizes, heat duties and operating conditions is given in Fig. 3. The relationship between the TAC and the vapor flow rate to the compressor is shown in Fig. 4. The vapor flow rate to the compressor plays a substantial role in the TAC analysis. As the vapor flow rate to the compressor increases, the TAC decreases gradually until achieving the lowest value. As the vapor flow rate to compressor increases further, the TAC increases at a

Table 3. Temperature control tuning parameters for basic control structure and improved structure

	Basic control structure CS1	Improved control structure CS2
Parameters	TC	TC
Controlled variable	T_{Lower4}	T_{Lower4}
Manipulated	Q_{RE}	Q_{RE}
Controller input range (°C)	0-242	0-242
Controller output range (GJ/hr)	0-4.015	0-4.015
Ultimate gain	1.11	1.37
Ultimate period (min)	4.2	4.2
Gain, K_C	0.347245	0.428998
Integral time, τ_I (min)	9.24	9.24

faster rate. The minimum TAC is 337666.75$ when the vapor flow rate to compressor is 2,340 kg/h.

To compare and analyze the comprehensive economic advantage of the SHPD technique, the conventional single-column distillation process is also given. Table 2 gives the economic results of the two processes. For the isopropanol and chlorobenzene separation, the TCC of SHPD process increases by 12.11×10^4 $ when compared with conventional single-column distillation. However, the SHPD conserves TOC of 21.48×10^4 $ and reduces TAC of 17.44×10^4 $ compared with the conventional single-column distillation.

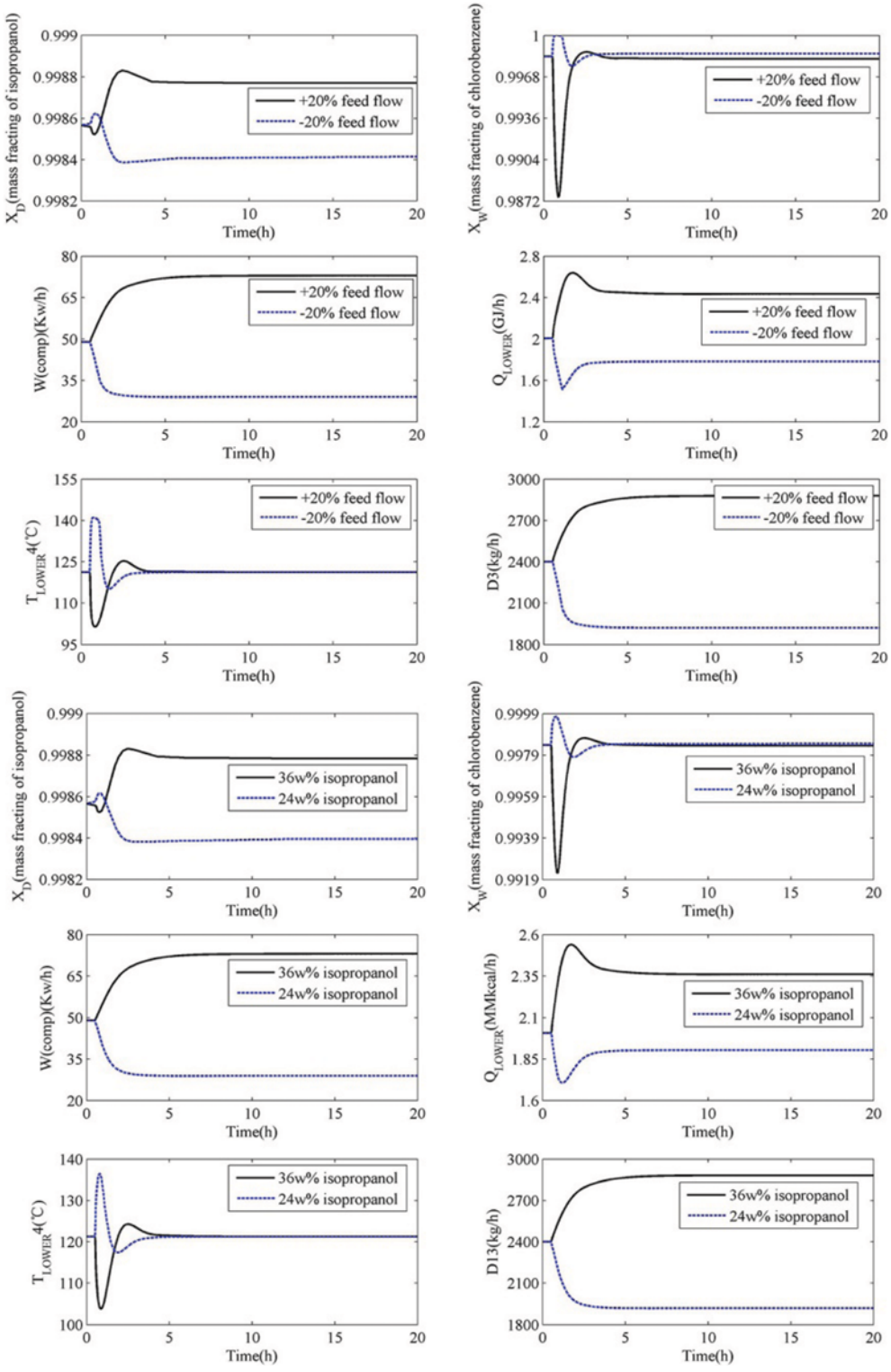

Fig. 7. Dynamic responses of the basic control structure.

CONTROL STRATEGY FOR THE SHPD

Before starting the dynamic simulation, the sizes must be specified for the plumbing system and major equipment, such as the column bases, reflux drum, etc. The volumes of reflux drum and column bases are specified to provide ~5 min of liquid holdup when half full by using the heuristic method. The ratios of height to diameter of the sumps and reflux drum are both set as 2. The diameters of the upper and lower column are calculated by the "Tray-Sizing" tool of Aspen Plus. All the pumps and values are inserted to give adequate pressure drops so that the control values drop enough pressure to handle changes in the flow rates with good range ability. Then the steady-state flowsheet is pressure-checked and the Aspen Plus file is exported to Aspen Plus Dynamics.

1. Selecting Temperature Control Tray

It is important to select the temperature control stage in a distillation column for the control structure. Fig. 5 shows the temperature and temperature difference profiles of the upper column and lower column. Tray temperature control is only considered for the lower column in the SHPD process, and the best temperature control locations on which the temperature has steep change from tray to tray was determined by slope criterion. Stage 4 shows a fairly steep slope in the SHPD and was selected as the temperature control stage.

2. Basic Control Structure for SHPD

The basic control structure and control panel are shown in Fig. 6 and the basic control schemes are as follows.

(1) Feed is flow-controlled (indirect acting).

(2) The level of the reflux drum is maintained by manipulating the flow of distillate flow (direct acting).

(3) Base level of the lower column is held by manipulating the flow of bottom product (direct acting). However, the base level of the upper column is held by manipulating the feed flow of the lower column (direct acting).

(4) The pressure in the upper column is maintained by manipulating the heat removal in the auxiliary condenser (indirect acting).

(5) D13 flow is flow-controlled (indirect acting). To achieve the constant of the mass reflux ratio, the D13 flow rate is cascaded with D10 flow rate by ratio control.

(6) UW3 flow is flow-controlled (indirect acting). To achieve the constant of the split fraction of the liquid splitter S2, the UW3 flow rate is cascaded with UW2 flow rate by ratio control.

(7) Material stream split fraction of the overhead vapor splitter is held by manipulating the brake power of the compressor (indirect acting).

(8) The temperature on stage 4 in the lower column is controlled by manipulating the reboiler heat input of the lower column (indirect acting).

(9) Deadtime of 1 min is inserted into the temperature control loop to reflect practical operation.

Conventional Proportional and Integral (PI) controllers are used for all controllers except the three liquid level controllers. Proportional controllers are used for all the level controllers with a gain of 2. The PI settings of the top pressure control loop for the upper column are set at K_C=20 and τ_I=12 min. The PI settings of the flow control loops are set at K_C=0.5 and τ_I=0.3 min. Relay-feedback test is run on the temperature controller to determine ultimate gains and periods, and the Tyreus-Luyben tuning rule is used in the tem-

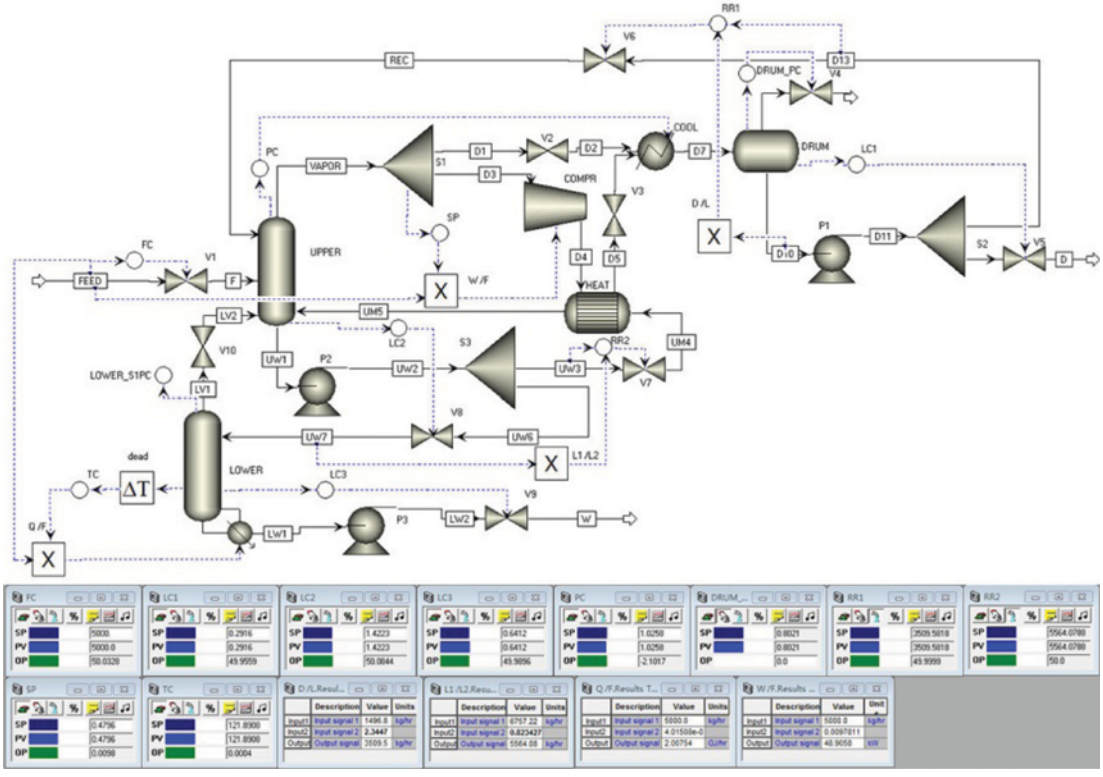

Fig. 8. Improved control structure.

perature controller. The tuning parameter for the temperature controller is shown in Table 3.

The dynamic performance of the basic control structure for the SHPD process was evaluated by feed flow rate and composition disturbances. Fig. 7 shows the dynamic results of the basic control structure to positive (solid lines) 20% and negative 20% (dashed lines) step changes in the feed disturbances at 0.5 h. The system can achieve a new steady state at 5 h after adding the feed disturbances, and the isopropanol purity and chlorobenzene purity come close to their set points and the controlled temperature arrives at the set point as

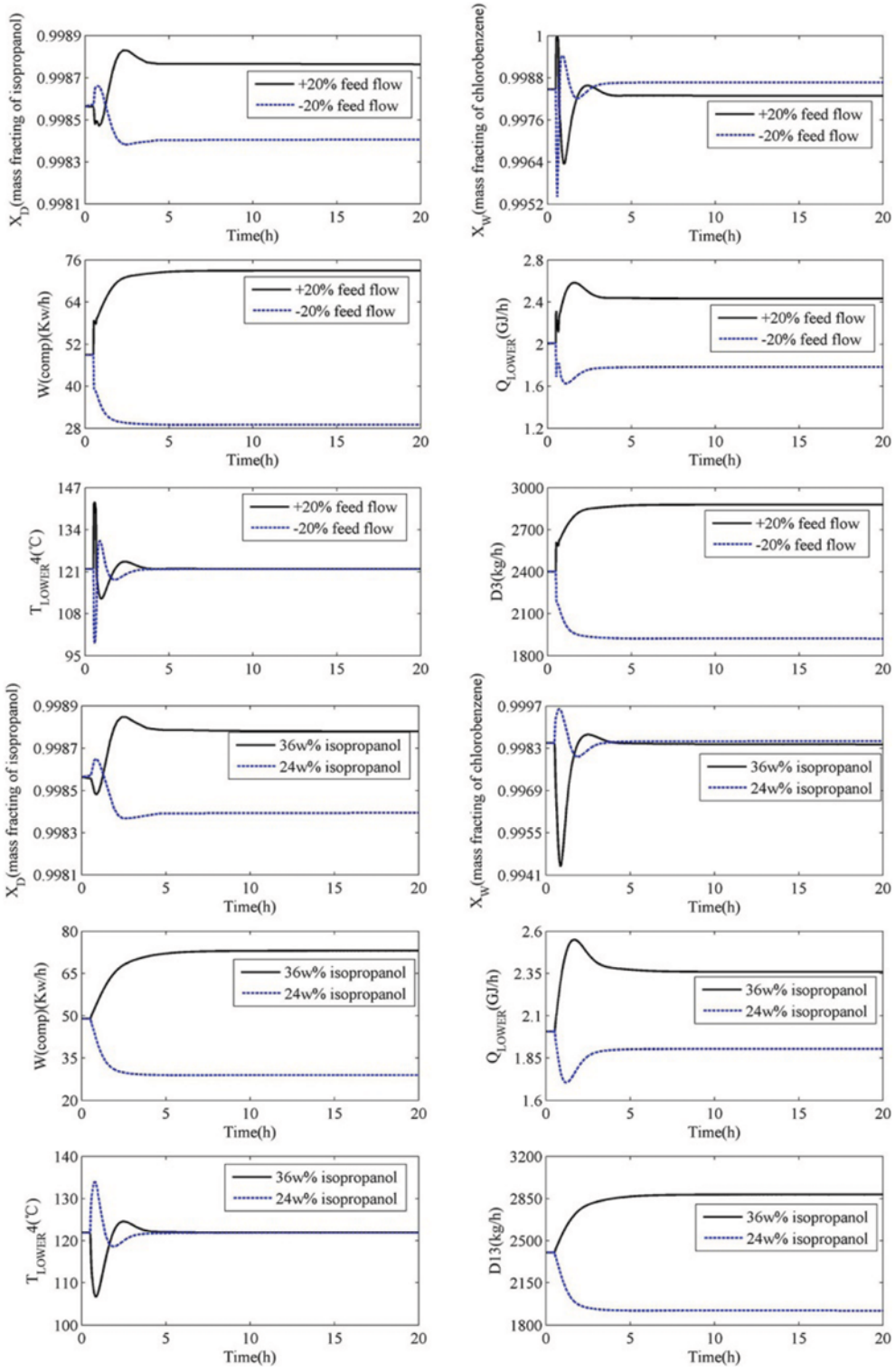

Fig. 9. Dynamic responses of the improved control structure.

well. However, the product purity of chlorobenzene has large transient deviation from the set point for introducing the positive 20% disturbances of feed flow rate, and the transient mass fraction of chlorobenzene is nearly 98.72 wt% when the feed flow rate increases. The reason is that the increased feed flow rate to the SHPD column eventually produces an immediate decrease in the isopropanol concentration at the bottom of the lower column according to the distillation principle, and the vapor flow rate controlled by the heat duty of the reboiler remains unchanged in a short time for the temperature controller with a big delay; that is, the mass fraction of chlorobenzene decreases very fast when the disturbances are introduced.

3. An Improved Control Structure for SHPD

The basic control structure cannot provide effective disturbance rejection for the 20% feed flow rate increase. The main reason is that the lower column heat input is not enough to produce sufficient vapor up to the top in time when the disturbance occurs, resulting in the large transient deviations of chlorobenzene product purity from the set point. A feedforward Q_{Re}/F ratio (lower column reboiler duty/feed flow rate) was adopted to improve the dynamic performance on the basis of the basic control structure. A feedforward W_m/F ratio (the brake power of compressor/feed flow rate) was also added in the improved control structure. The tuning parameter for the temperature controller of improved structure is also shown in Table 3. Fig. 8 illustrates this improved control structure and controller faceplates.

Fig. 9 demonstrates the dynamic results for the improved control structure by adding ±20% feed flow rate and feed composition disturbances. The improved control structure gives better control with shorter settling time and smaller peak transient deviations. The system comes to a new steady state within 4 h, and the product purities are kept close to the set points, which are acceptable levels of quality. The largest transient deviation of the chlorobenzene product purity reduced from 0.011 to 0.002 for +20% feed flow rate when two feedforwards Q_{Re}/F ratio and W_m/F control scheme were inserted. This is because a rapid increase heat input to the lower column reboiler when +20% feed flow rate occurs and then promotes the more isopropanol component escaping from the bottom.

Consequently, the improved control structure can adjust operational parameters more rapidly to obtain better dynamic performances than basic control structure in face of feed rate flow and composition disturbances.

CONCLUSION

A method for the separation of isopropanol/chlorobenzene mixture was developed using SHPD technology. Rigorous steady state and dynamic performance for this process were simulated using Aspen Plus and Aspen Plus Dynamics. The optimal design for the SHPD process was obtained with the objective function of TAC minimization. This optimal flowsheet of the SHPD process was compared with conventional single-column distillation, and the result shows that the SHPD process has an obvious economic advantage.

Two control structures were presented and examined for this SHPD process in face of ±20% feed flow rate and composition disturbances. The basic control structure had large transient deviations when +20% feed flow rate disturbance occurred. Improved control structure with feed forward control was adopted to get a more robust control. The dynamic responses show that the improved control structure has shorter settling time and smaller fluctuation than the basic control structure.

This study has shown that the SHPD process is worth considering for separating the binary mixture which has a larger relative volatility in the low composition range than in the high composition range.

ACKNOWLEDGEMENT

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NOMENCLATURE

SHPD : separate heat pump distillation
TAC : total annual cost
TOC : total operating cost
TCC : total capital cost
C_S : reboiler of the lower column
C_{CW} : cooling water for the auxiliary condenser
C_{Ele} : electricity for the compressor
C_{CV} : column vessel cost
C_{HE} : heat exchangers cost
C_{Comp} : compressor cost
TC : temperature controller of column
PI : proportional and integral
K_C : gain of controller
τ_i : integral time of controller
Q_{Re}/F : lower column reboiler duty/feed flow rate
W_m/F : the brake power of compressor/feed flow rate

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