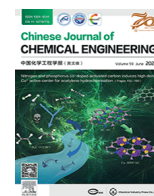




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Full Length Article

A dynamic control structure of liquid-only transfer stream distillation column

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ABSTRACT

The intention of this fundamental work is to explore the manipulation of a mixture of benzene, toluene and *o*-xylene separated from liquid-only transfer divided-wall column (LTS-DWC). First, two control structures are clearly proposed, including seven component control loops (CS1) and seven temperature control loops (CS2). However, two control structures can handle $\pm 10\%$ feed disturbances rather than larger feed disturbances. Subsequently, an equivalent four-column model by introducing withdraw ratio is developed to discuss the effect of two liquid-only side-stream on the overall reboiler duty. It is indicated that the second liquid-only side-stream withdraw ratio strongly affects the overall energy consumption. Hence, six-component control loops within the fixed second liquid-only side-stream withdraw ratio (CS3) is proposed and the purity of products returns to set value even as facing $\pm 20\%$ feed disturbances. Finally, based on the above results, it is established a temperature control structure (CS4) for controlling fixed second liquid-only side-stream withdraw ratio, which can cope with $\pm 15\%$ disturbances. Inspired by these findings, an insight into the dynamic control of LTS-DWC promotes the industrial implementation of DWC through new liquid-only side-stream configurations.

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1. Introduction

Divided-wall column (DWC) enables efficient separation of three-component mixtures, which effectively avoids the remixing of intermediate components and takes advantage of its thermodynamic advantages [1–5]. This thermally coupled structure ensures that the separation takes place in the same column, which reduces not only energy consumption but also capital costs.

There's a growing recognition that the dynamic control of DWC is still challenging for the industrial implementation of DWC due to various controlled and manipulated variables (such as reboiler duty (Q_R), reflux ratio (RR), side product flow rate (S), liquid split ratio (β_L), and vapor split ratio (β_V)) [6]. Kiss *et al.* [7] explored some kinds of DWC control strategies to separate BTX mixture and found that the liquid, side stream and vapor boil-up rate (LSV), distillate, side-stream and boil-up (DSV) are capable of handling persistent impacts in short times. In order to operate under minimum energy consumption, the prefractionator composition

of the heaviest component can be controlled by operating the liquid split ratio to separate out the BTX mixture in the DWC [8]. Yuan and Skogestad *et al.* [9,10] studied four control structures to operate the light impurity ethanol in the side-stream. It is indicated that three temperature control strategy (CS1) is better than control strategies (CS2, CS3, CS4) with the addition of a component control board with a fixed vapor split ratio. Huang *et al.* [11] clearly proposed simplified temperature differential control (STDC), which combines temperature control and temperature differential control for separating ethanol, propanol, and butanol in DWC. Subsequently, the dual temperature differential structure (DTDC) is proposed, whose dynamic control performance is much more effective than that of temperature differential control [12]. It can cope well with 30% of feed composition disturbances. For the large feed oscillations in Kaibel DWC (KDWC), a working pressure compensation temperature control structure within an active vapor split ratio is explicitly proposed to manipulate the purity of the downstream product, which contributes potential solutions for dynamic operation of KDWC in industrial [13]. Obviously, among the five manipulated variables of DWC, β_V and β_L play a crucial role in the optimal control of DWC [14–18]. In industrial, it is relatively easy to control the β_L through collectors and distributors during

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operation column [19]. The β_V cannot be manipulated in industrial production, since the vapor split ratio is constrained by cross-section and the pressure drops on both sides of the diaphragm when the position of the partition is determined in DWCs. Although active steam dispensers are invented for better industrial application of DWC [20], such as external steam diversion device [21], and vane shaped steam distribution devices [22], the dynamic control of DWCs with fixed vapor split ratio is proposed for the majority of studies [8,9,23–25], except little literature to separate multi-component mixture in experimental DWC [26]. For instance, Dwivedi *et al.* [16] verified the feasibility of vapor split ratio as a variable with temperature control structures in a self-built four-column experimental setup. Li *et al.* [18] proposed a new hydraulically driven steam splitter that satisfies the gas distribution needs of industry.

Agrawal [27] proposed a method to reduce the original vapor split ratio depending on the addition of one or more steam distillation stages and reboilers and condenser. A new liquid-only transfer divided-wall column (LTS-DWC) structure using liquid-only transfer stream, which is thermodynamically equivalent to a conventional DWC, but avoids operation difficulties of vapor split flow streams in the conventional DWC. The LTS-DWC greatly reduces the operational implementation difficulties and opens a huge scope for industrial applications of DWCs [28,29]. Recently, Ge *et al.* [30] investigated the structure and operating parameters of the four products DWC (FPDWC) by a sequential optimization method and analyzed the equivalence of the new configuration with the original configuration while extending to the space of the FPDWC with two dividing walls. Sun *et al.* [25] explored the concentration and temperature control scheme of LTS-DWC. According to the ratio of the duty of the reboiler to the total flow of the side stream, the dynamic control structure of the link where the C2 xylene concentration value changes the most after the oscillation is manipulated, and a good practical effect is obtained in the BTX system software. All commodity ingredients can be repaired to the required purity with small errors. Subsequently, Sun *et al.* [31] proposed an optimal design of the Kaibel column (KC)-LTS suitable for BTXH quaternary distillation. It is discovered that the control structure that the heavy composition is controlled by boil-up/side-stream flow achieved good dynamic control at $\pm 20\%$ disturbances. It is worth noting that rare efforts have been made to study the optimal design and control of LTS-DWC presently. However, previous LTS-DWC dynamic control studies show fewer control schemes with reboiler duty as an operating variable. The more in-depth influence of two liquid-only side-stream on dynamic control performance of LTS-DWC under large feed disturbances is absent.

In this work, four control structures are proposed for the dynamic control of LTS-DWC for separating benzene, toluene, and *o*-xylene mixture. Firstly, seven-component control loops (CS1) and seven-temperature control loops (CS2) are developed for controlling LTS-DWC. It is discovered that the dynamic control performance of CS1 is the same as CS2, however two control structures can handle $\pm 10\%$ feed disturbances rather than larger feed disturbances. Hence, an equivalent four-column model by introducing withdraw ratio is developed to discuss the effect of two liquid-only side-stream on the overall energy consumption duty. It is indicated that the second liquid-only side-stream withdraw ratio strongly affects the overall energy consumption. Therefore, CS3 that includes six component control loops within the second liquid-only side-stream withdraw ratio is proposed and the purity of products returns to set value even as facing $\pm 20\%$ feed disturbances. On the base of CS3, a temperature control structure CS4 within fixed second liquid-only side-stream withdraw ratio is proposed, which can resist $\pm 10\%$ or $\pm 15\%$ feed disturbances.

2. Steady State Design of LTS-DWC

There are seven operating freedom degrees for the LTS-DWC, which are the reboiler duty (Q_{R1} , Q_{R2}), return flow rate (R_1 , R_2), two liquid flows transferred between the two columns (L_1 , L_2), and side-stream S . The conventional DWC optimization methods aim at the minimum total annual cost (TAC). The economic accounting basis of the TAC objective function is shown in Table S1 (see Supplementary Material). For the steady-state design of the LTS-DWC, reference is made to the multi-objective genetic algorithm, which is one of the steady-state optimization design methods of DWC [32–34]. It is set up in such a way that the total number of stages in both columns is equal. The LTS-DWC configuration is shown in Fig. S1, with the decision variables (number of stages per fraction) marked. N_1 to N_6 represent the number of stages in each part of the column, which does not include the reboiler and condenser. Eventually, their relationship is qualified:

$$N_1 + N_3 + N_5 = N_2 + N_4 + N_6 \quad (1)$$

A ternary composition of benzene (B), toluene (T), and *o*-xylene (X) is studied with boiling points of 353, 385, and 419 K for the three components at atmospheric pressure. The feed flow rate and temperature are set at $3600 \text{ kmol} \cdot \text{h}^{-1}$ and 358 K, respectively. A molar ratio of 3:3:4 is considered for each component. The simulation is performed by using the Aspen Plus V11. The rigorous calculation module Radfrac is used for the simulation, and the physical method is CHAO-SEAD. All products are specified to be extracted at 99% (mol). The LTS-DWC configuration is obtained on the base of the basic configuration of the divided-wall column (DWC). It is optimized by MATLAB multi-objective genetic algorithm. Finally, it is obtained the relationship between the total column stages and the reboiler heat duty, as shown in Fig. S2. It is calculated the TAC for each LTS-DWC configuration.

The comparison of DWC and LTS-DWC is displayed in Table S2. It is found that LTS-DWC is nearly equal to the dividing wall distillation column in terms of energy consumption, which would be slightly higher economically due to the double-column design. Total economic cost saves 19% and total duty saves 30.4% compared to conventional distillation processes.

The optimized results are given in Fig. 1. LTS-DWC configuration contained two columns with only liquid flow transfer between the two columns. The first distillation column (C1) contains two product flows and the second distillation column (C2) contains three product flows. The component and temperature distributions of the two columns are shown in Fig. S3. In C1, B shows a monotonically decreasing variation, and T shows two back mixing above and below the feed stage. In C2, B was basically completed in the 15th stage. The temperature difference between top and bottom of distillation column is always maintained at 80 K.

3. Dynamic Control Structure of LTS-DWC

3.1. Component control structure of LTS-DWC CS1

The component control of the LTS-DWC is the same as for basic distillation equipment, where the operating variables are adjusted according to the impurity concentration in the column stage or in the product withdraw stream. In this contribution, PID controllers are used for the dynamic control. The control scheme of CS1 is illustrated in Table 1. The component control flow chart in Fig. 2 contains a total of seven control loops, including four control loops for C1 and three control loops for C2. Each control loop has 5 min dead time. Because the reboiler heat duty has the most direct impact on the whole column control variables, the priority is

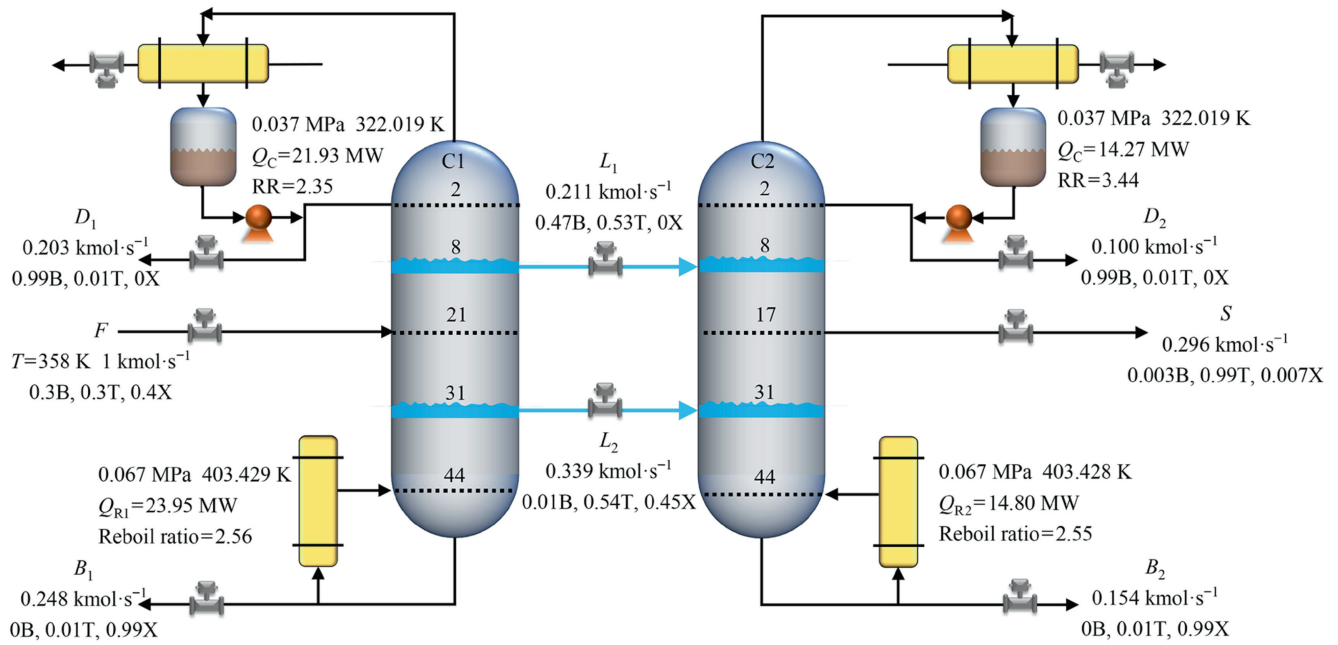


Fig. 1. Liquid-only transfer stream distillation column flow chart.

Table 1
Controller tuning parameters for CS1

Control loop	Controlled variable	Manipulated variable	Controller gain K_c	Controller integral time τ_i/min
CC1	$x_{D1}(T)$	R_1	0.06	86.80
CC2	$x_{L1}(X)$	L_1	0.05	67.32
CC3	$x_{L2}(B)$	L_2	0.05	91.08
CC4	$x_{B1}(T)$	Q_{R1}	0.04	52.80
CC5	$x_{D2}(T)$	D_2	0.14	122.76
CC6	$x_S(X)$	S	0.06	47.52
CC7	$x_{B2}(T)$	Q_{R2}	0.05	46.20

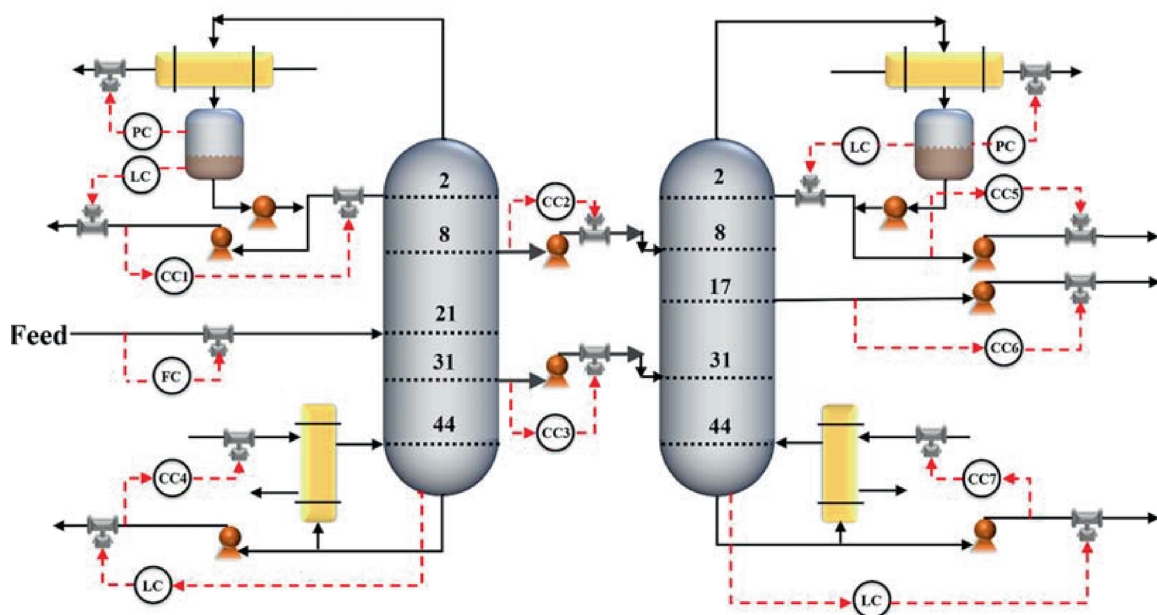


Fig. 2. Component control structure (CS1) for LTS-DWC.

$Q_{R1}/x_{B1(T)}$. The return flow has a greater impact on the whole column control variables, so the second is $R_1/x_{D1(T)}$ and the last are $L_1/x_{L1(X)}$ and $L_2/x_{L2(B)}$ loops. The order of building control loops for C2 is the same as C1, and the last is $S/x_{S(X)}$ loop. And the relay test is carried out to obtain the proportional gain value and integration time using the Tyreus–Luyben method. Then all parameters are obtained and shown in Table 1.

In order to better assess the effectiveness of the control structure, the information characteristics of the CS1 are assessed based on the introduction of $\pm 10\%$ total feed flow and compositional disturbances. The disturbances to the process are given at 1 h. Fig. 3 depicts the dynamic response of LTS-DWC due to $\pm 10\%$ disturbances of the feed flow rate and composition, with the other components scaled. It is observed that the concentrations of the product are basically controlled at around 99.0% within about 15 h. However, compared with feed composition disturbances, the purity of C2 commodity fluctuates greatly and the initial setting time is longer. Because in LTS-DWC steady-state design, once the flow rate changes significantly, it is difficult to cope with the reboiler heat duty of C2 with minimum energy consumption. It is considered to sacrifice some energy consumption and expand its operation range to make it cope with the fluctuation of flow rate change.

3.2. Temperature control structure of LTS-DWC CS2

In the classical two-component distillation separation process, the temperature has a one-to-one correspondence with composition at a constant operating pressure. In C1, R_1 , L_1 , L_2 , and Q_{R1} are considered as the manipulated variables for the temperature in sensitive stages, while D_2 , S , and Q_{R2} are utilized as manipulated variables for temperature control loops in C2.

Singular value decomposition (SVD) method is applied to find out the sensitive stage. The sensitive stages of the two columns are obtained, as shown in Fig. 4. Noteworthy, the open-loop

steady-state gain between the temperature of the fifth plate and the return flow rate of C1 is large. According to the principle of close pairing, the temperature of the fifth plate can be effectively controlled by the return flow rate of C1. Besides, the distribution of benzene and toluene composition before and after the fifth plate varies widely (see Fig. S3). When facing the feed disturbance, the return flow rate of C1 controls the temperature of the fifth plate unchanged, which can maintain the composition distribution of this tower section and realize the separation of benzene and toluene. Therefore, the controlled variable corresponding to the return flow rate of C1 is the temperature of the fifth plate. It is determined that the sensitive stages of C1 are the fifth ($T_{C1,5}$) (1 for distillation column 1, 5 for stage 5), sixteenth ($T_{C1,16}$), twenty-fourth ($T_{C1,24}$), and thirty-ninth ($T_{C1,39}$), and the sensitive stages of C2 are the seventh ($T_{C2,7}$), twenty-fourth ($T_{C2,24}$), and thirty-ninth ($T_{C2,39}$). Hence, $T_{C1,5}$, $T_{C1,16}$, $T_{C1,24}$, and $T_{C1,39}$ are controlled by R_1 , L_1 , L_2 , and Q_{R1} , respectively in C1. $T_{C2,7}$, $T_{C2,24}$, and $T_{C2,39}$ are controlled by R_2 , S , and Q_{R2} , respectively in C2.

Fig. 5 depicts the control scheme of CS2 for LTS-DWC. As shown in this figure, the tuning order of temperature controllers is TC4 (C1 column bottom), TC1 (C1 column top), TC2 (C1 upper sideline), TC3 (C1 lower sideline), TC7 (C2 column kettle), TC5 (C2 column top), and TC6 (C2 sideline). Table 2 lists each temperature controller parameters after successful tuning and the dead time of each controller is 1 min. The dynamic response of CS2 in face of $\pm 10\%$ composition and feed flow rate disturbances are demonstrated in Fig. 6. Apparently, the purity of each product of C2 oscillates more dramatically and has more stabilization time compared with that of C1. Furthermore, the majority of the product purity does not return to their optimal values ($\pm 0.3\%$) after about 10 h. In addition, the dynamic control characteristics of CS2 are better than CS1. Although there is a strong oscillation compared with CS1, the purity of each product under CS2 will eventually be restored to $\pm 10\%$ oscillation of the design value. However, both CS1 and CS2 cannot handle larger feed disturbances ($\pm 20\%$).

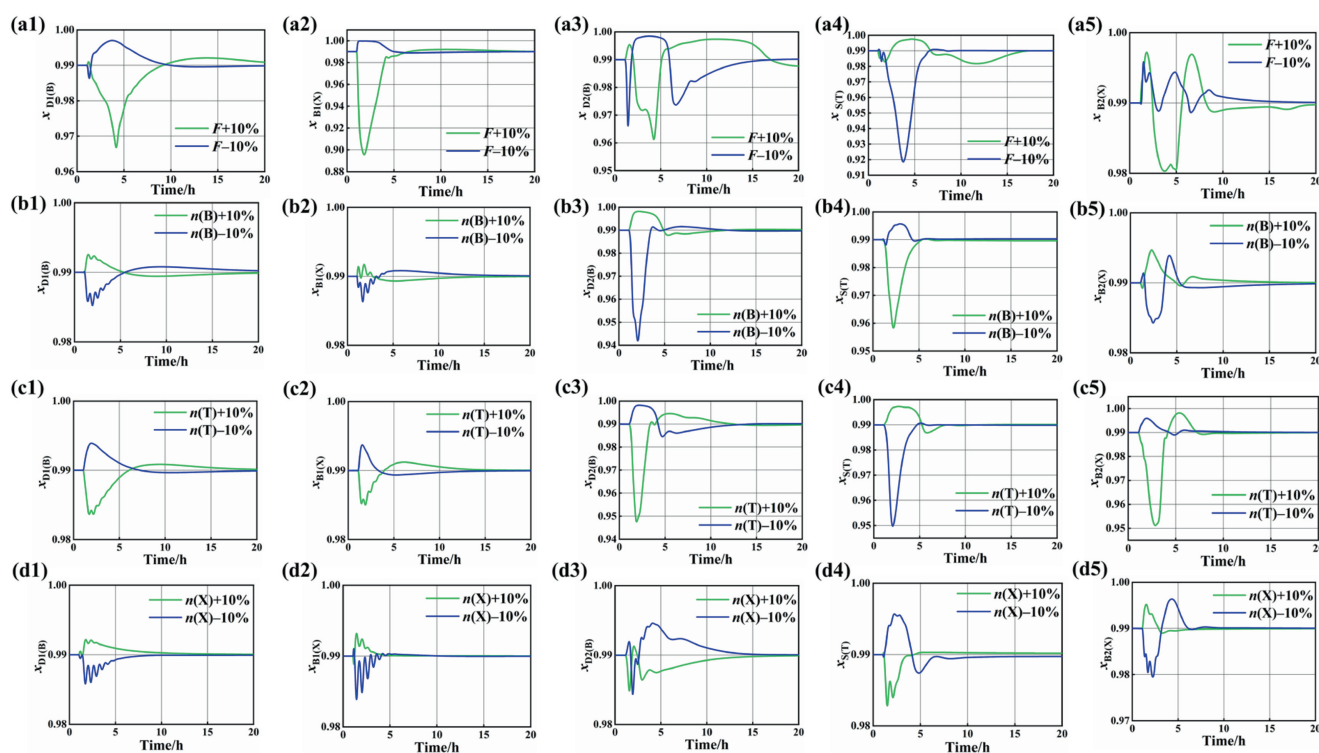


Fig. 3. Variations of product concentration under CS1: (a) $\pm 10\%$ feed flow rate disturbance, (b) $\pm 10\%$ benzene composition disturbance, (c) $\pm 10\%$ toluene composition disturbance, (d) $\pm 10\%$ xylene composition disturbance.

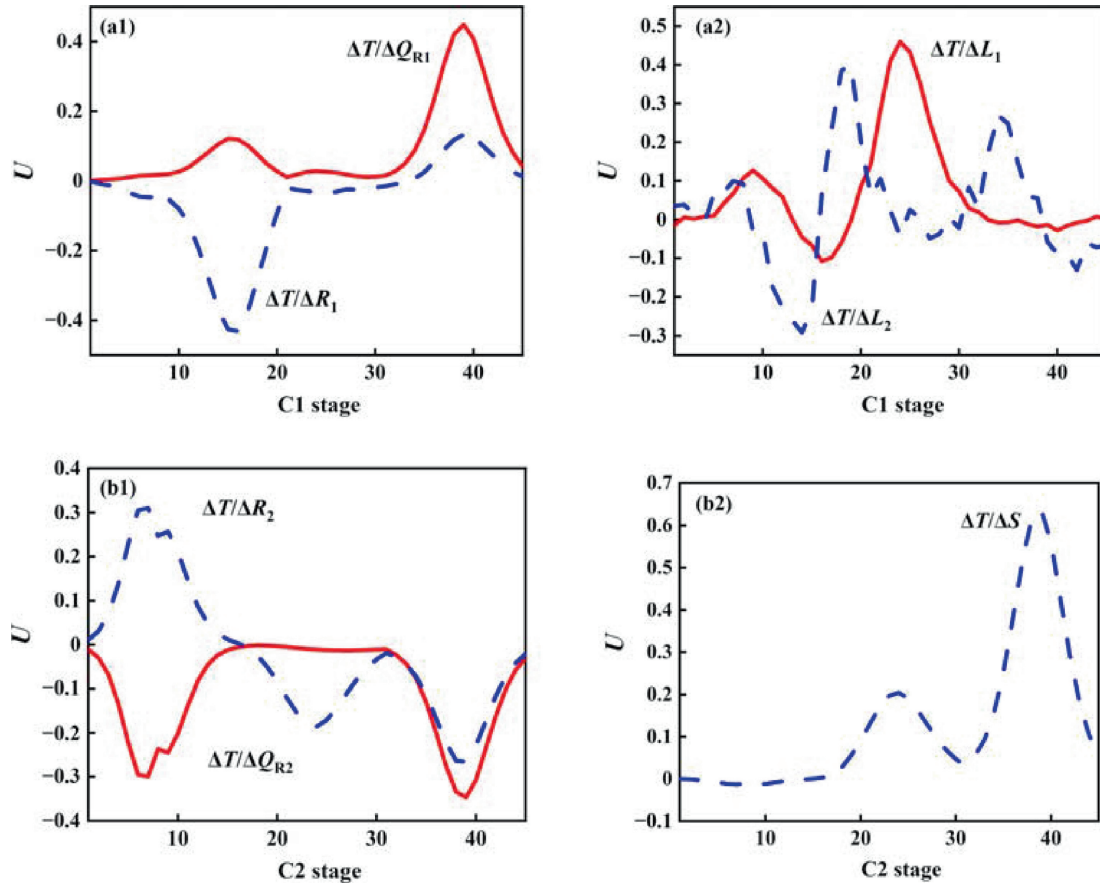


Fig. 4. Methods of single value decomposition analysis for (a) C1 and (b) C2.

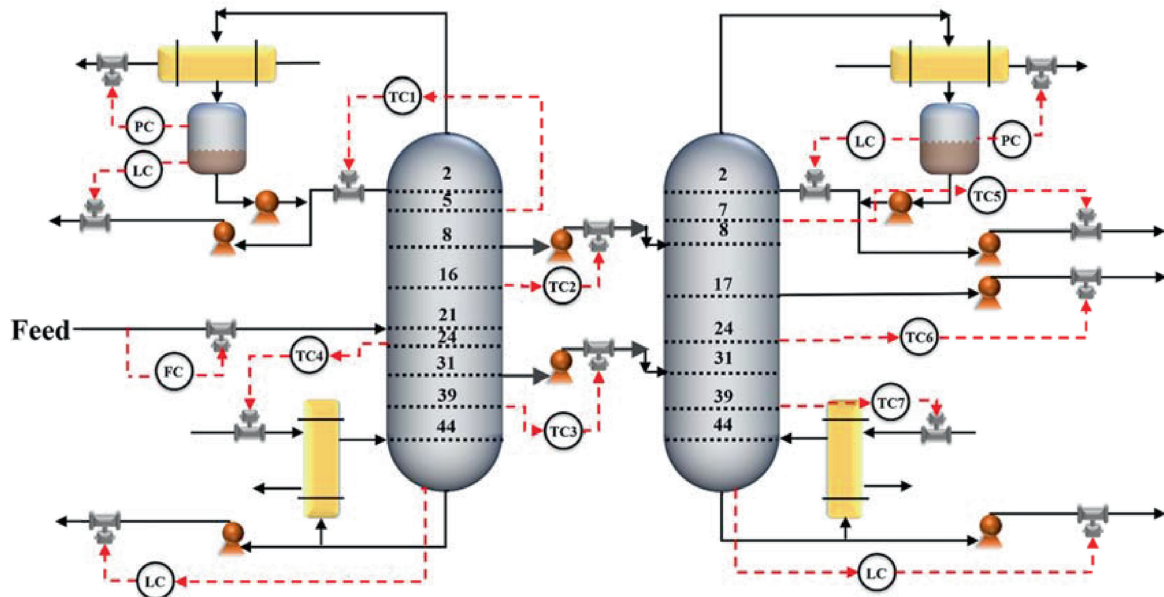


Fig. 5. Temperature control structure (CS2) for LTS-DWC.

3.3. Component control structure of equivalent four-column CS3

It is mentioned above that the advantage of LTS-DWC is that only the liquid phase is transferred throughout the column, which is easier to achieve and more controllable in industry than traditional DWC. Meanwhile, the two liquid side streams have a signif-

icant impact not only on the steady-state design but also on the dynamic control, which was rarely discussed in previous literature, especially the withdraw ratio of the two liquid side streams (withdraw flow L_i /total flow TL_i). Hence, an equivalent four-column model of the LTS-DWC is proposed (see Fig. 7), where the original C1 in LTS-DWC is subdivided into three distillation columns C11,

Table 2
Controller tuning parameters for CS2

Loop	Controlled variable	Manipulated variable	Controller gain K_C	Controller integral time τ_i/min
TC1	$T_{C1,5}$	R_1	2.83	13.20
TC2	$T_{C1,16}$	L_1	3.43	23.76
TC3	$T_{C1,39}$	L_2	7.79	17.16
TC4	$T_{C1,24}$	Q_{R1}	2.69	9.24
TC5	$T_{C2,7}$	D_2	4.65	34.32
TC6	$T_{C2,24}$	S	4.22	18.48
TC7	$T_{C2,39}$	Q_{R2}	2.75	7.92

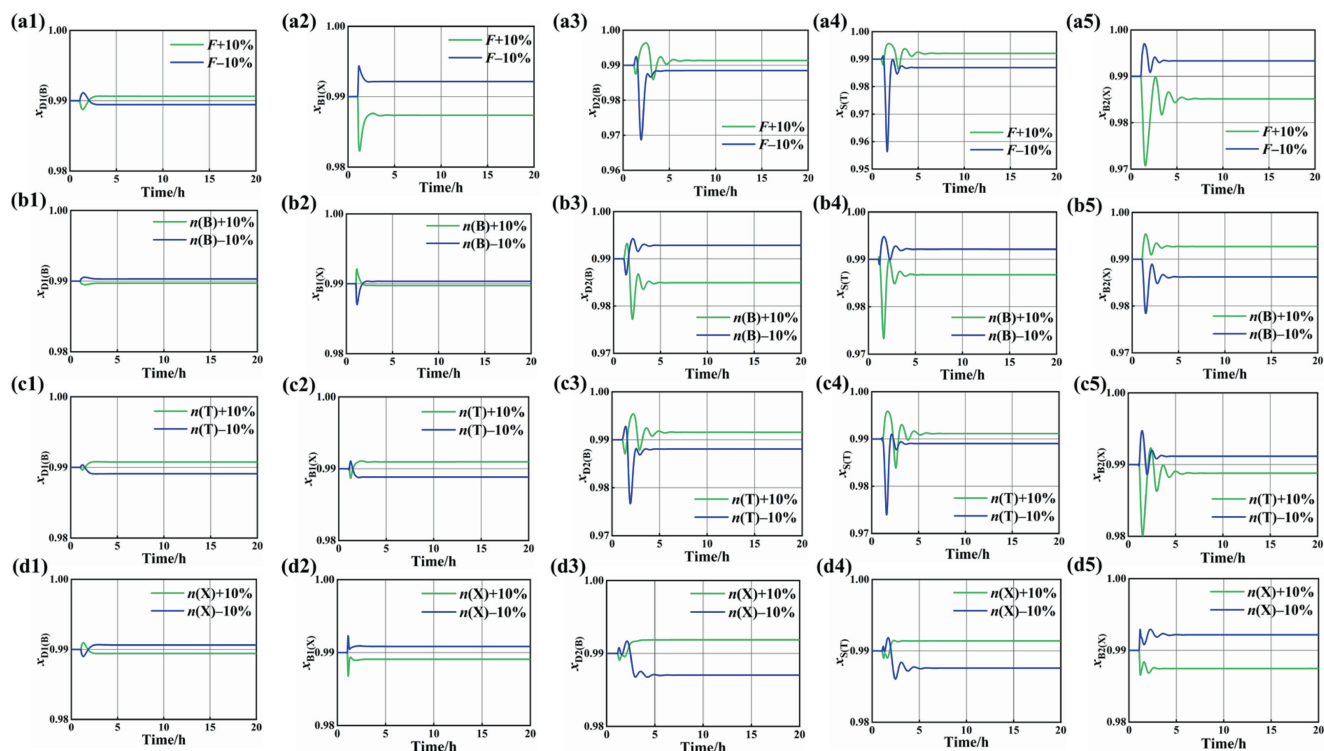


Fig. 6. Variations of product concentration under CS2: (a) $\pm 10\%$ feed flow rate disturbance, (b) $\pm 10\%$ benzene composition disturbance, (c) $\pm 10\%$ toluene composition disturbance, (d) $\pm 10\%$ xylene composition disturbance.

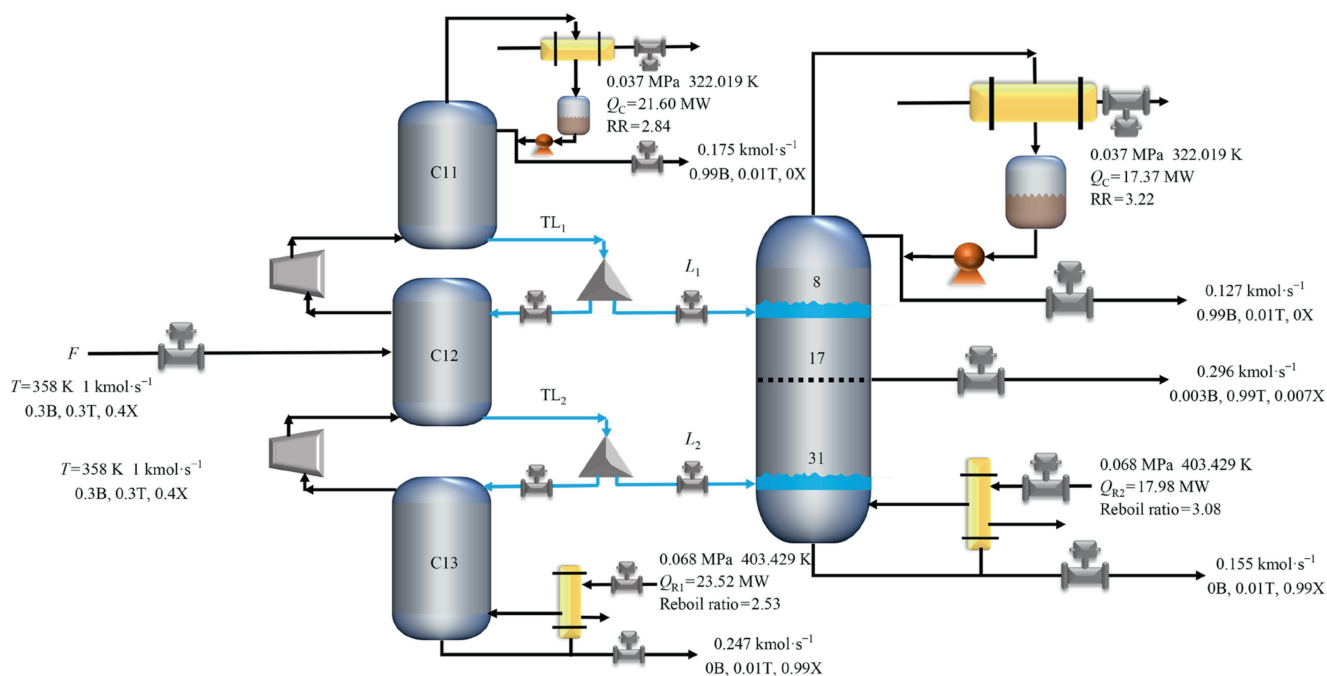


Fig. 7. Equivalent four-column model flow chart.

C12 and C13 with two splitters. This model is thermodynamically equivalent to the LTS-DWC. There are 7 stages in C11, 23 stages in C12, and 15 stages in C13, where the first liquid commercial stream from the C11 column is split into C12 and C2 by a splitter, and the

second liquid stream from the C12 column is split into C13 and C2. The detailed parameters of the equivalent four-column model are illustrated in Fig. 7. For instance, the column pressure of C11 and C₂ is 0.0375 and 0.058 MPa, respectively. Furthermore, the with-

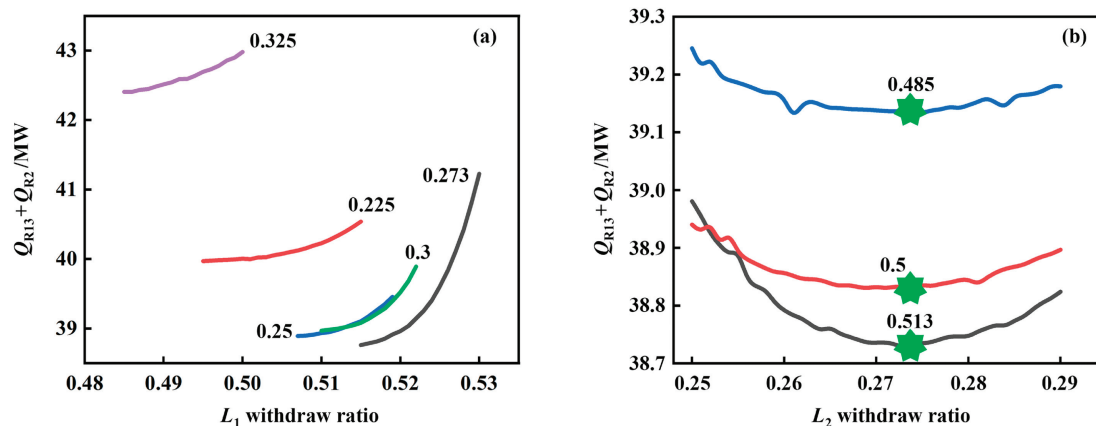


Fig. 8. Equivalent four-column reboiler input at different withdraw ratios.

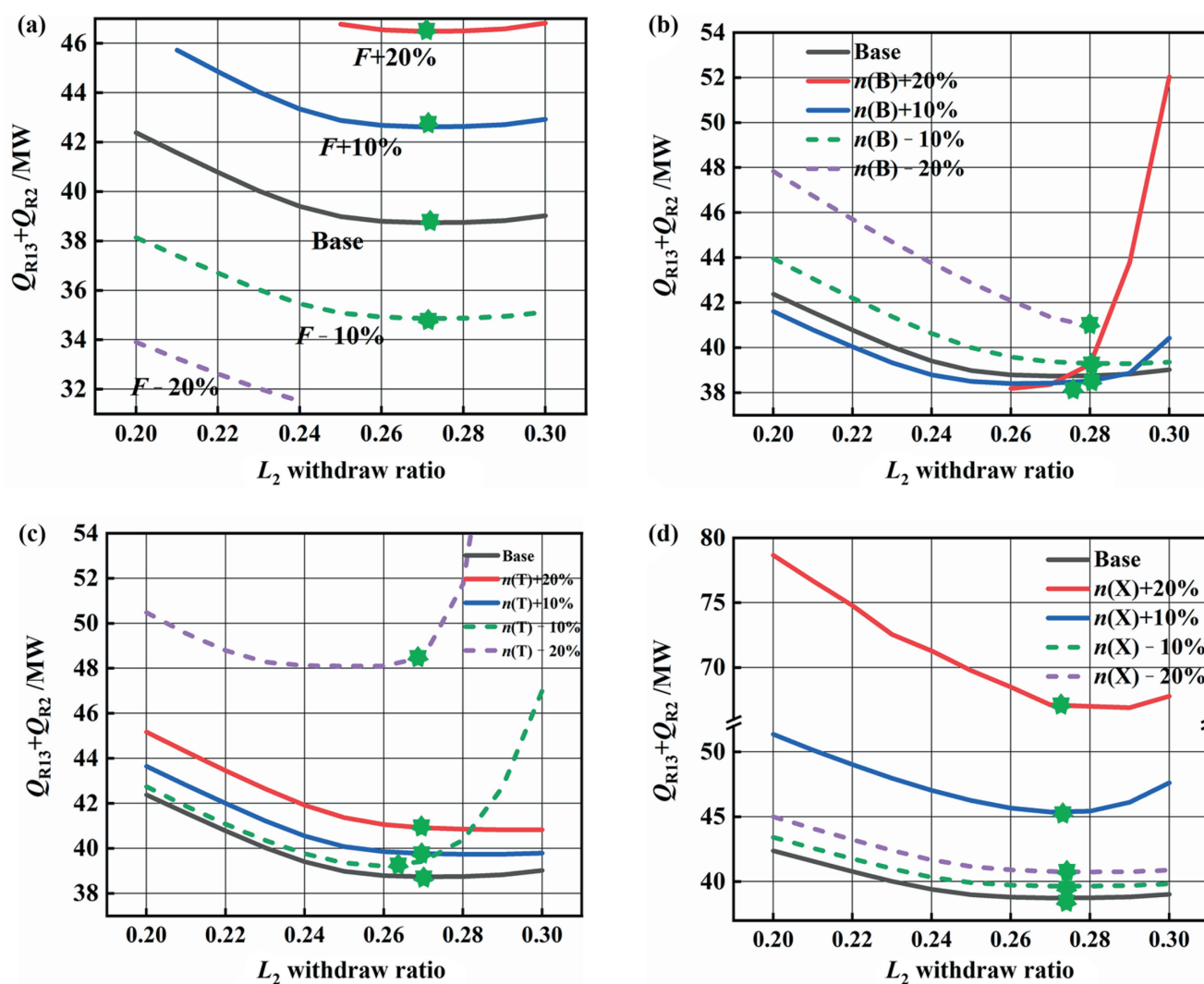


Fig. 9. (a) L_2 withdraw ratio on heat duty for changes under flow feed changes, (b) L_2 withdraw ratio on heat duty for changes under benzene feed changes, (c) L_2 withdraw ratio on heat duty for changes under toluene feed changes, (d) L_2 withdraw ratio on heat duty for changes under xylene feed changes.

draw ratio of L_1 is 0.513 (L_1/TL_1), and the withdraw ratio of L_2 is 0.273 (L_2/TL_2).

Apparently, increasing either withdraw ratio will lead to decrease C13 reboiler duty and increase C2 reboiler duty, while decreasing either withdraw ratio will also lead to increase C13 reboiler duty and decrease C2 reboiler duty. In order to evaluate the combined effect of withdraw ratios of L_1 and L_2 on the overall energy consumption, various withdraw ratios of L_1 and L_2 are considered in the equivalent four-columns. The impact of withdraw ratios of L_1 and L_2 on overall energy consumption is revealed in Fig. 8. It is observed that the energy consumption of the equivalent four-columns increases with the increase of L_1 withdraw ratio within fixed L_2 withdraw ratio, and the steady-state structure cannot meet the design requirement when L_1 withdraw ratio increases to a certain value. In Fig. 8(b) the total boiler duty development trend decreases first and then increases when L_1 withdraw ratio is fixed and L_2 withdraw ratio is active. The optimized L_2 withdraw ratio when a minimum reboiler duty is achieved is 0.273.

Fig. 9 demonstrates the effect of L_2 withdraw ratio on overall heat duty of LTS-DWC under different feed conditions. It is observed that various feed conditions exhibit similar trends of overall energy consumption. The heat duty of LTS-DWC first decreases and then increases with the improvement of L_2 with-

draw ratio. Furthermore, the optimized L_2 withdraw ratio for different feed conditions is approximately 0.273 (see asterisk marks in Fig. 9), which indicates that the control of L_2 withdraw ratio is crucial when facing larger disturbances of feed conditions. Hence, an improved control structure CS3 is proposed that the L_2 withdraw ratio of C12 is set as manipulated variable (see Table 3). Meanwhile, a multiplier module is used in this structure. The total flow from C12 is the first signal. Secondly, the ratio of the input flow into C13 to the total flow is another signal (see Fig. 10). Fig. 11 depicts the dynamic performance of CS3 as facing $\pm 20\%$ feed disturbances, respectively. Obviously, the dynamic response of CS3 is superior to that CS1 and CS2 even in the face of larger feed disturbances. The purity of all products returns to designed value within about ten hours, which indicates the effectiveness of controlling the withdraw ratio in LTS-DWC.

3.4. Temperature control structure of equivalent four-column CS4

Due to the thermodynamic equivalence of the equivalent four-columns with the LTS-DWC, the temperature sensitive stages are selected with reference to the SVD results of the LTS-DWC. According to the control structure of component control CS3, R_{11} , L_1 , L_2 ,

Table 3
Controller tuning parameters for CS3

Loop	Controlled variable	Manipulated variable	Controller gain K_C	Controller integral time τ_I/min
CC1	$x_{D1}(T)$	R_{11}	0.14	55.44
CC2	$x_{L1}(X)$	L_1	0.05	97.68
CC3	$x_{B1}(T)$	Q_{R13}	0.05	54.12
RC	Withdraw ratio	L_2	0.5	0.3
CC4	$x_{D2}(T)$	R_2	0.05	99.00
CC5	$x_S(X)$	S	0.06	55.44
CC6	$x_{B2}(T)$	Q_{R2}	0.05	54.12

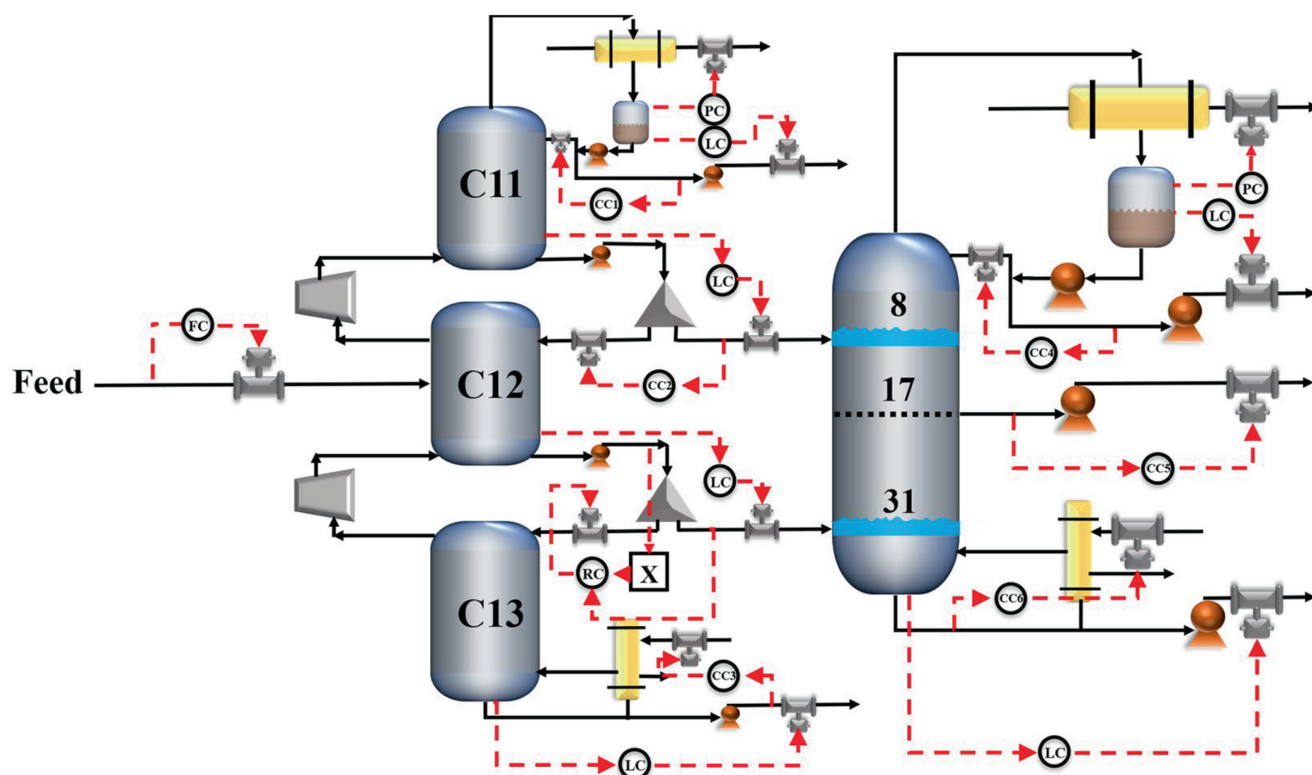


Fig. 10. Component control structure with withdraw ratio (CS3) for equivalent four columns.

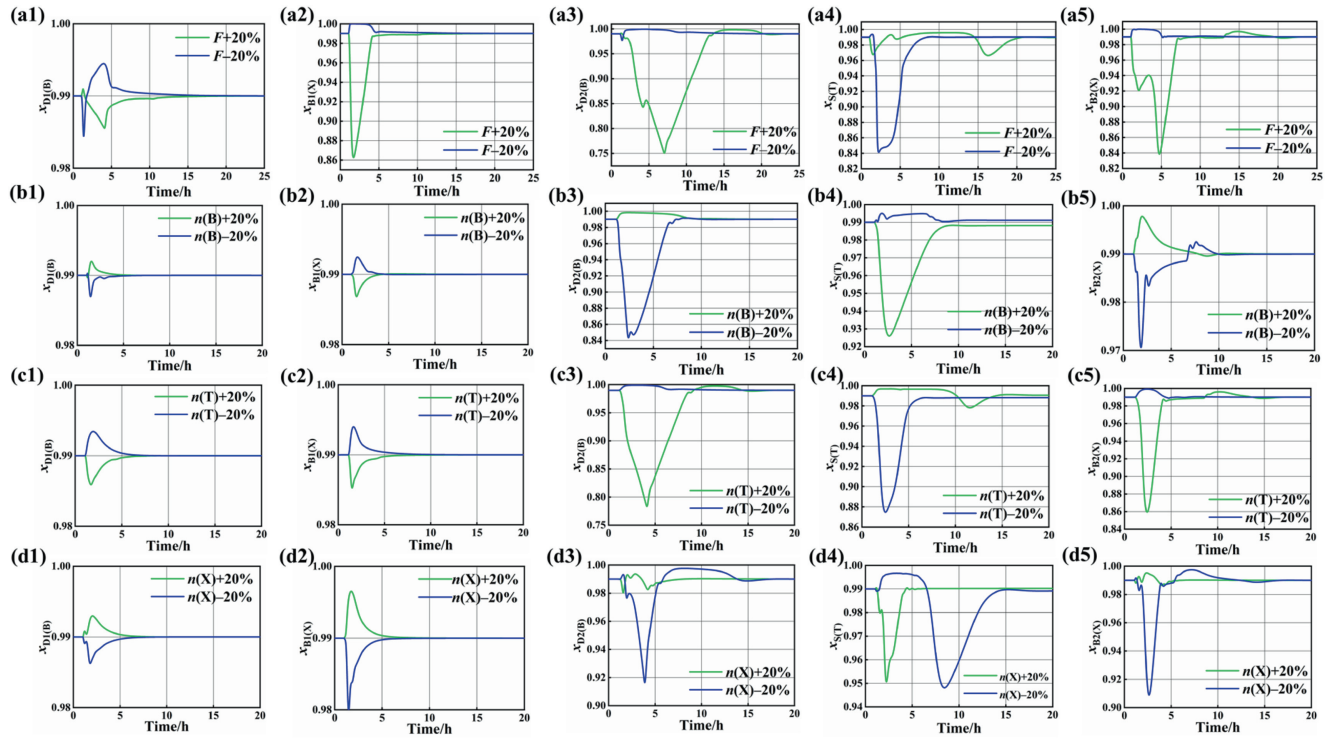


Fig. 11. Variation of product concentration under CS3: (a) $\pm 20\%$ feed flow rate disturbance, (b) $\pm 20\%$ benzene composition disturbance (c) $\pm 20\%$ toluene composition disturbance, (d) $\pm 20\%$ xylene composition disturbance.

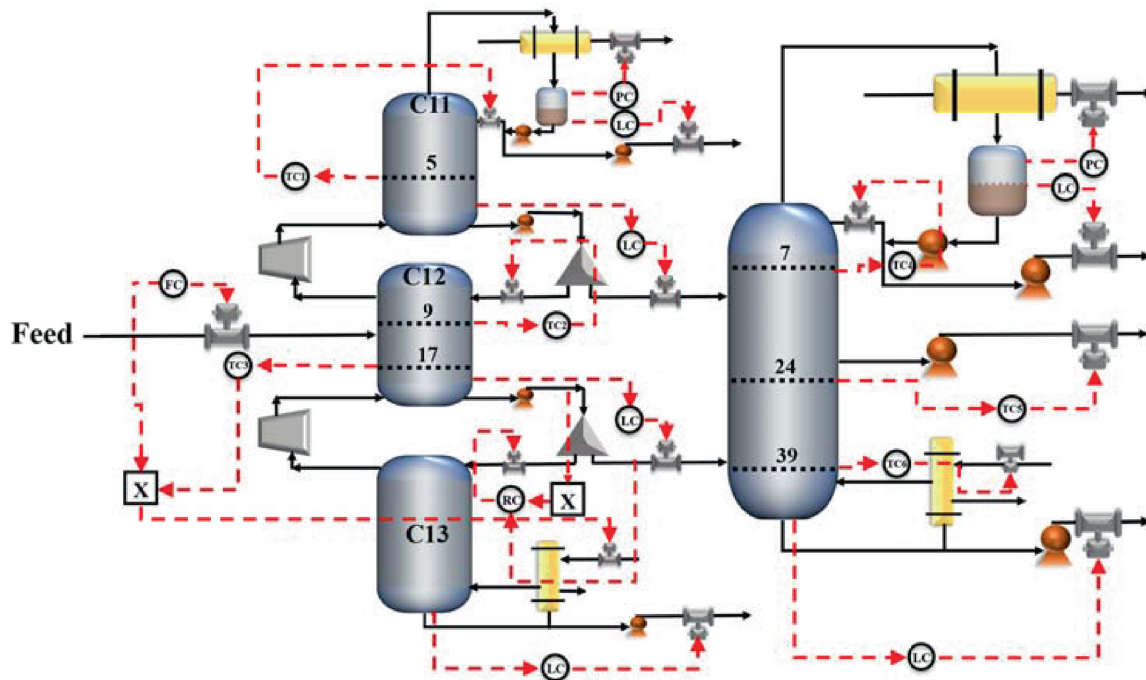


Fig. 12. Temperature control structure (CS4) for equivalent four columns.

Q_{R13} are used to control $T_{C11,5}$, $T_{C12,9}$, L_2 extraction ratio, $T_{C12,17}$, and R_2 , S , Q_{R2} are used to control $T_{C2,7}$, $T_{C2,24}$, $T_{C2,39}$. CS4 with fixed L_2/F extraction ratio is shown in Fig. 12. To better control the purity of the product at the bottom of the C13, a proportional control of L_2/F is added to the control structure. The tuning sequence is the same as other control structures, and the specific tuning parameters are shown in Table 4. As shown in Fig. 13, the variation of each

product purity for $\pm 10\%$ and $\pm 15\%$ disturbances of the feed flow or component is examined, where the dashed line represents the $\pm 10\%$ product concentration variation and the solid line represents $\pm 15\%$. Overall, CS4 shows good control results in face of severe disturbances in feed flow or components. Compared to CS3, CS4 reduces smoothing time and vibration amplitude and CS4 is easier to implement in industry.

Table 4
Controller tuning parameters for CS4

Loop	Controlled variable	Manipulated variable	Controller gain K_C	Controller integral time τ_I/min
TC1	$T_{C11,5}$	R_{11}	4.69	10.56
TC2	$T_{C12,9}$	L_1	4.47	23.76
TC3	$T_{C12,17}$	Q_{R13}	2.56	19.80
RC	Withdraw ratio	L_2	0.5	0.30
TC4	$T_{C2,7}$	R_2	1.32	23.76
TC5	$T_{C2,24}$	S	4.56	21.12
TC6	$T_{C2,39}$	Q_{R2}	3.12	7.92

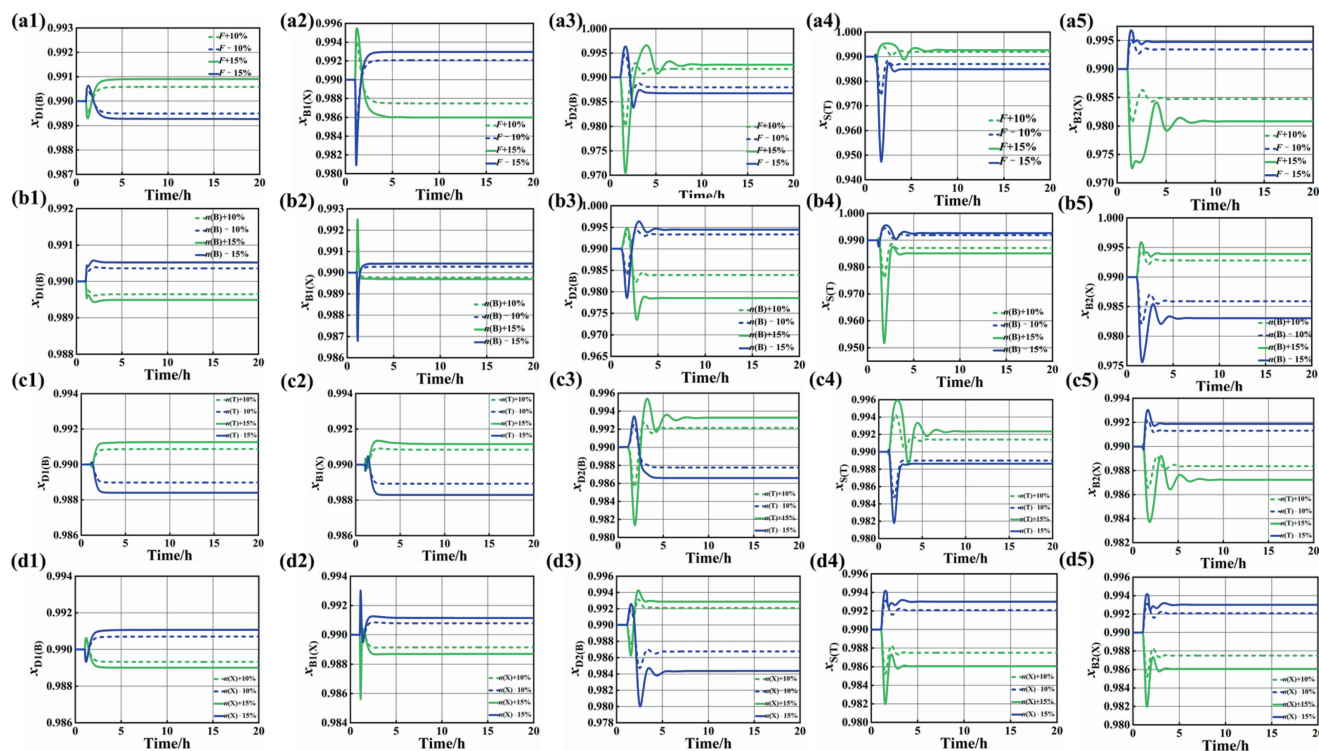


Fig. 13. Equivalent four-column feed flow and composition disturbance $\pm 10\%$ and $\pm 15\%$ product purity for CS4 control structure.

4. Conclusions

The dynamic control of LTS-DWC for separating benzene, toluene and *o*-xylene mixtures is discussed. First, seven-component control loop CS1 and seven-temperature control loop CS2 are proposed. It is observed that as facing $\pm 10\%$ disturbances that the purity of each product under CS2 eventually recovers to the design value despite the dramatic oscillations compared with CS1. Meanwhile, two control schemes cannot handle larger feed disturbances ($\pm 20\%$). Subsequently, an equivalent four-columns model by introducing withdraw ratio is developed to discuss the effect of two liquid-only side-stream on the overall reboiler duty. It is indicated that the second liquid-only side-stream withdraw ratio strongly affects the overall energy consumption. Hence, six-component control loops within the second liquid-only side-stream withdraw ratio (CS3) is proposed and the purity of products returns to set value even as facing $\pm 20\%$ feed disturbances. Finally, CS4 temperature control structure can cope with $\pm 15\%$ of the feed flow or component disturbances and is more suitable for industrial distillation processes.

Data Availability

Data will be made available on request.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary Material

Supplementary material to this article can be found online at <https://doi.org/10.1016/j.cjche.2022.12.009>.

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