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Comparison of Alternative Control Systems of Reactive Distillation Columns with Top-Bottom External Recycle

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Reactive distillation columns with external recycle between the top and bottom (RDCs-TBER) have a better steady-state performance as compared with conventional reactive distillation columns (CRDCs) for the separations of reacting mixtures featuring the most unfavorable ranking of relative volatilities (i.e., the reactants are the lightest and heaviest components with the generated products in between). In this article, the dynamics and control of RDCs-TBER are studied in great detailed. Three control systems (CSI, CSII, and CSIII) are developed for RDCs-TBER. CSI utilizes the reboiler heat duty and the side draw flow rate to control the composition of the side draw product C and the bottom level, respectively, and the external recycle flow rate is kept constant. CSII is the same as CSI except that the reboiler heat duty and the side draw flow rate are used to control the bottom level and the composition of the side draw product C, respectively. CSIII adapt from CSII by adding a control loop that the external recycle flow rate is employed to control the composition of the side draw product D. A reactive distillation system, executing a hypothetical reversible reaction, A + B ↔ C + D ($\alpha_A > \alpha_C > \alpha_D > \alpha_B$), is employed to inspect the dynamics and controllability of the RDC-TBER. The results showed that the CSII and CSIII have better dynamic performance than the CSI. In additional, the supplementary manipulated variable (i.e., the flow rate of the external recycle) can be used to improve the process operation.

1. Introduction

For the separation of reacting mixtures featuring the most unfavorable ranking of relative volatilities (i.e., the reactants are the lightest and heaviest components with the generated products in between), it is difficult to achieved high product purities with conventional reactive distillation columns (termed as CRDCs, hereinafter, Chen et al., 2013). To deal this issue, Tung and Yu (2007) proposed a kind of reactive distillation columns with two reactive sections at the top and bottom (RDC-TRS) and the products are withdrawn as side draw. Despite the specific configuration can acquire high product purity, a huge energy consumption should be applied. In order to overcome this difficulty, we proposed to adding an external recycle between the top and bottom and/or utilizing feed splitting technology to enhance the internal mass integration and internal heat integration of reactive distillation column and thus derived five kinds of process alternatives with feed splitting and/or external recycle (Chen et al, 2016): (i) reactive distillation columns with two reactive sections and feed splitting (termed as RDC-TRS-FS, hereinafter); (ii) RDC-TRS-FS with external recycle (termed as RDC-TRS-FS-ER, hereinafter); (iii) reactive distillation columns with two reactive sections and external recycle (termed as RDC-TRS-ER, hereinafter); (iv) reactive distillation columns with a top-bottom external recycle (termed as RDC-TBER, hereinafter); (iii) RDC-TBER with feed splitting (termed as RDC-TBER-FS, hereinafter). The results showed that adding a top-bottom external recycle and/or utilizing feed splitting technology to the reactive distillation column can largely improve the steady-state system performance as compared with the RDC-TRS and the CRDC for the separations of reacting mixtures featuring the most unfavorable ranking of relative volatilities. Although the researches on the steady state showed that the two methods employed have great advantages on enhancing process thermodynamics efficiency, their dynamics and controllability are needed to be studied.

In terms of the dynamics and control of RDC-TRS-FS for separating a two-stage consecutive reacting mixture (A + B ↔ C + D, C + B ↔ E + D with $\alpha_D > \alpha_B > \alpha_C > \alpha_A > \alpha_E$), Kaymak et al. (2017) provided four types of control structures including a temperature inferential control, a direct composition control, and two hybrid temperature and composition control and concluded that the last two control schemes can achieve effective control performance with little steady state deviations. Lately, Cao et al. (2017) found that deliberate arrangement and control of feed splitting can give great favorable effects on process dynamics and control. As for the dynamics and control of RDC-TBER (c.f. Figure 1b), few papers can be found to the best of our knowledge, even though it has comparable (or even better) steady state performance than RDC-TRS-FS in some reaction systems. The RDC-TBER have more manipulating valuable (i.e., the flow rate of external recycle) than the CRDC because of the process retrofitting, which means that the RDC-TBER might have improved dynamic performance than the CRDC with the operation of the flow rate of external recycle even though the former represents much stronger internal mass integration and internal heat integration than the latter. Therefore, researches on the effects of external recycle to process operation and control are necessary. The main purpose of the current article is to gain insights into the dynamic behaviors of the RDC-TBER and develop effective control systems. Detailed comparisons are made between the three control systems for the RDC-TBER. The separations of a hypothetical ideal quaternary reaction is employed as illustrative example to evaluate the impact of external recycle on process dynamics and control. After a brief discussion of the obtained outcomes, the article ends with the conclusions that can be drawn.

2. Dynamics and control of RDC-TBER

As sketched in Figure 1a, the RDC-TBER for the separation of the most unfavorable reacting mixtures (exothermic reaction) is configured in such a way that the reactive section is arranged deliberately at the bottom (which include not only the reboiler but also some stages in the lower section divided by the stage for withdrawing the reaction products). The lightest reactant A and the heaviest reactant B are fed, respectively, into the reboiler and at the top of the reactive section with the light product C and the heavy product D withdrawn together as an intermediate product above the reactive section. An external recycle is arranged from the top to the bottom. It is noted that this arrangement leaves the RDC-TBER in a totally totally reboiled operation mode. Three control systems (CSI, CSII, and CSIII, shown in Figure 1b, 1c, and 1d) are developed for RDCs-TBER. They are: (1) CSI: the reboiler heat duty control the composition of the side draw product C, the side draw flow rate control the bottom level, the reflux control the top level, the heaviest reactant feed flow rate control the B composition of the sensitive stage to keep the stoichiometric proportion, and the external recycle flow rate is kept constant; (2) CSII: the side draw flow rate control the composition of the side draw product C, the reboiler heat duty control the bottom level, the reflux control the top level, the heaviest reactant feed flow rate control the B composition of the sensitive stage to keep the stoichiometric proportion, and the external recycle flow rate is kept constant; (3) CSIII: the side draw flow rate control the composition of the side draw product C, the reboiler heat duty control the bottom level, the reflux control the top level, the heaviest reactant feed flow rate control the B composition of the sensitive stage to keep the stoichiometric proportion, and the external recycle flow rate control the composition of the side draw product D.

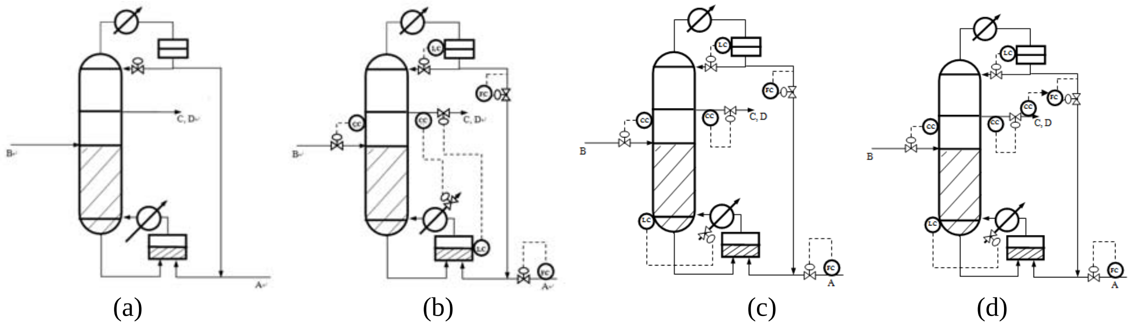


Figure 1. RDC-TBER and its control system designs: (a) RDC-TBER, (b) CSI, (c) CSII, (d) CSIII

First, the regulation path is to be analyzed. For CSI, the control loops of side product, bottom level, and stoichiometric proportion are strong interconnected. Specifically, once the composition of the products increases, the reboiler heat duty would increase, which lead the decrease of the bottom level. Then, the side draw flow rate decreases, which lead the increase of the composition of the side draw product C. Therefore, the strong interconnection of the three control loops makes the tuning of the controller complicated and control performance would be deteriorated. For CSII and CSIII, varying the side draw flow rate could not directly affect the compositions of the intermediate product. Its variation should do this job though the bottom inventory control loop; that is, the variation of the side draw flow rate will affect the level of the bottom, then the reboiler heat duty would be adjusted, and then the compositions of the intermediate product will change indirectly. The specific arrangement of the control system attenuates the interconnection between the control loops as compared with CSI, and the augment operating variable (i.e., external recycle flow rate) can be used to enhance the control performance of the CSIII.

Second, the disturbance path is to be analyzed. For CSI, once the lightest feed flow rate increases, the bottom level increases and the side draw flow rate should decrease, which lead the composition of the side draw product C increases and the B composition of the sensitive stage decreases. Then, the reboiler heat duty should decreases, which lead the increase of the bottom level. Therefore, the strong interconnection of the three control loops makes control performance deteriorated. For CSII and CSIII, the interconnection between the control loops is also attenuated as compared with CSI. The external recycle flow rate can be utilized to control the composition of the side draw product D, which can enhance the control performance of the CSIII

In the following, a reactive distillation system for the separation of a hypothetical reversible reaction, A + B↔C + D ($\alpha_A > \alpha_C > \alpha_D > \alpha_B$) is used to examine the insights on the dynamics and controllability of the RDC-TBER.

3. An illustrative example: A hypothetical ideal exothermic reaction

3.1 Process Studied

As shown in Figure 2, the two reactive distillation systems, i.e., the CRDC and RDC-TBER, are taken from Chen et al. (2013), which separate a hypothetical reversible exothermic reaction.

A + B ↔ C + D (1)

The detail operating conditions of the illustrative example are shown in Table 1. To save the space, the main physicochemical properties are omitted and one can found them in the relevant reference. The commercial software Mathematica is used in process simulation. In comparison with the CRDC, the RDC-TBER reduces the reboiler heat duty largely, highlighting the great potential of external recycle in process revamp.

Table 1. Operating Conditions of the Illustrative Example

Parameter		Value
Product specification (mol %)	C	47.5
	D	47.5
Relative volatility A:B:C:D		8:1:4:2
Heat of reaction (kJ/kmol)		–20920
Total number of stages		32
Number of reactive stages (including reactor/condenser/reboiler)		12
Reactive holdup per reactive stage (kmol)		4
Reactive holdup on reboiler/reactor (kmol)		80
Reboiler duty (MW)		5.121

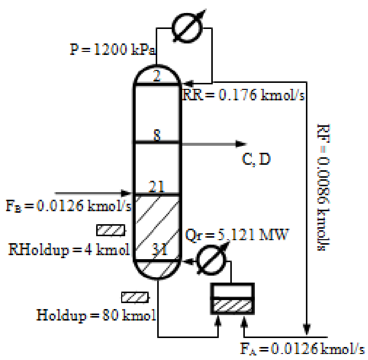


Figure 2. Process synthesis and design of RDC-TBER

3.2 Open-Loop Dynamic Characteristics

Figures 3a and 3b depict the open-loop responses of the CSI after they encounter +5% step disturbances in the lightest feed flow rate, respectively (In this paper, open-loop means that all the control loops are open while the two level loops are close). For both the positive and the negative perturbations, the RDC-TBER shows seriously under-damped responses in the C and D compositions of the intermediate product. It is noted that the C composition of the intermediate product competes intensively with the D composition of the intermediate product, giving rise to quite similar responses but with opposite changing directions. For the CSII, step disturbances in the lightest feed flow rate cannot be used to evaluate the open-loop performance because side draw flow rate control loop is open and the feed flow rate disturbance will lead the system unstable. Note that the CSIII has the same control configuration as the CSII. Figure 3c and 3d show the open-loop responses of the CSII (CSIII) after +5% step changes are introduced into the A feed composition (i.e., pure A change into 0.95A and 0.05B). Note that the under-damped phenomenon is restrained as compared to CSI.

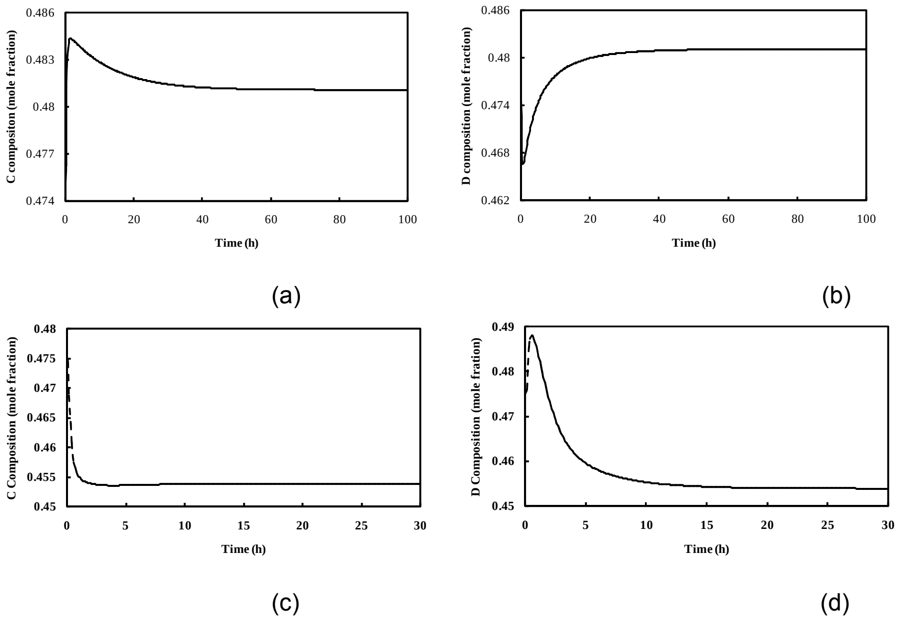


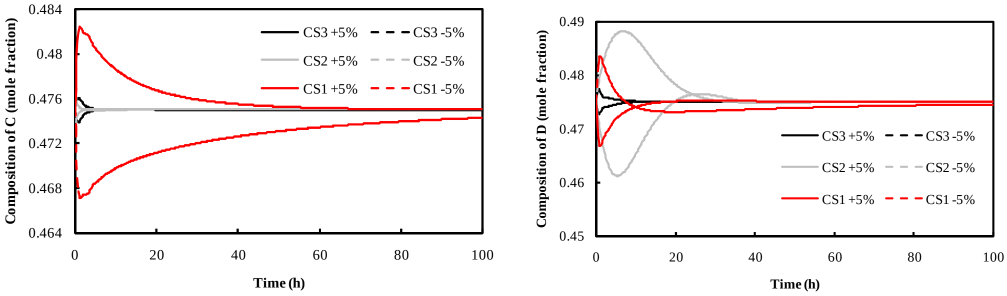
Figure 3. The open-loop responses of the RDC-TBER. (a) C composition for CSI, (b) D composition for CSI, (c) C composition for CSII(CSIII), (d)D compostion

3.3 Closed-Loop Operation

Direct composition control schemes are employed here as shown in Figure 1b, 1c, and 1d. Column pressure is regulated with the condenser heat removal, and the inventories of the reflux drum and reboiler are regulated with the reflux and reboiler heat duty, respectively, via a P-only controller. The product compositions are controlled with two methods. One is that the C composition of the intermediate product is regulated by the intermediate product flow rate via a PI controller, leaving the D composition of the intermediate product uncontrolled (c.f. Figure 4a); and the other is that the C composition of the intermediate product is regulated by the intermediate product flow rate and the D composition of the intermediate product is regulated by external recycle flow rate (c.f. Figure 4b). The B feed flow rate is employed to control the composition of B on stage 10 in the RDC-TBER since the composition variation is the largest at this stage, serving to keep the stoichiometric ratio between the lightest reactant A and the heaviest reactant B. Although a P-only composition controller or a PI composition controller can be used here, for the sake of simplicity, the former option is chosen. The A feed flow rate is flow-controlled and works as the production rate handle. The composition controllers, designed in-line with the Tyreus− Luyben tuning rule. Composition measurement devices are assumed to act like a first order process with a 3 min time constant, and control valves are all set at the half-open position in the nominal steady state. The controller tuning parameters are shown in Table 2.

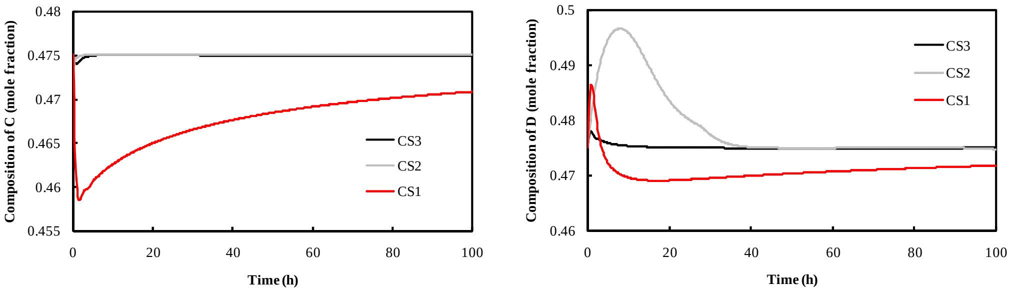
Table 2. Controller Parameters for the three control systems

	CSI		CSII		CSIII	
Control loop	K_C(-)	T_I(min)	K_C(-)	T_I(min)	K_C(-)	T_I(min)
Top level	2	-	0.5	-	0.5	-
Composition at sensitive stage	0.001	-	0.001	-	0.0005	240000
C composition	1818	5398	1.36	3000	0.68	6000
Bottom level	0.008	-	40	-	40	-
D composition	-	-	-	-	0.4	4500



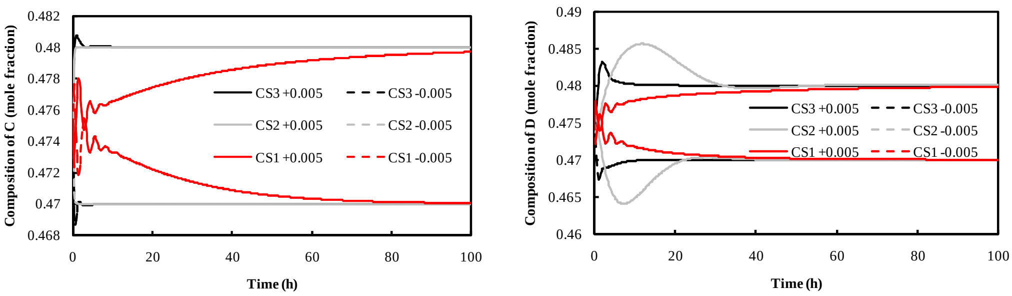
(a) (b)

Figure 5. The regulatory responses of the three control systems after ±5% step changes are introduced into the A feed flow rate



(a) (b)

Figure 6. The regulatory responses of the three control systems after -5% step changes are introduced into the A feed composition



(a) (b)

Figure 7. The regulatory responses of the three control systems after ±0.005 step changes are introduced into the product composition

The regulatory responses of the three control systems are illustrated in Figure 5, 6, and 7 after ±5% step changes are introduced in the A feed flow rate, -5% step change in the A feed composition, and ±0.005 step changes in the product composition, respectively. The results showed that CSII and CSIII are found to be advantageous over the CSI and the control performance of the RDC-TBER can be enhanced largely with the manipulating of external recycle.

4. Conclusions

Three control systems are developed to study the dynamics and control of RDCs-TBER. One utilizes the reboiler heat duty and the side draw flow rate to control the composition of the side draw product C and the bottom level, respectively, and the external recycle flow rate is kept constant. The second one uses the reboiler heat duty and the side draw flow rate to control the bottom level and the composition of the side draw product C, respectively. The last one adapt from the second one by adding an control loop of the external recycle flow rate controlling the composition of the side draw product D.

The reactive distillation system carrying out a hypothetical reversible exothermic reaction has been employed to scrutinize the dynamics and control of the RDC-TBER. The obtained results have confirmed that with the adoption of external recycle the RDC-TBER helps to substantially enhance the system control performance.

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