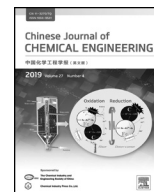




Contents lists available at ScienceDirect

Chinese Journal of Chemical Engineering

journal homepage: www.elsevier.com/locate/CJChE

Article

Temperature inferential control of a reactive distillation column with double reactive sections[☆]Lijing Zang, Kejin Huang^{*}, Ting Guo, Yang Yuan, Haisheng Chen, Liang Zhang, Xing Qian, Shaofeng Wang

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ARTICLE INFO

Article history:

Received 18 September 2018

Received in revised form 18 November 2018

Accepted 27 November 2018

Available online 11 December 2018

Keywords:

Reactive distillation column

Temperature inferential control

Sensitivity analysis

Transient deviation

Steady-state deviation

ABSTRACT

Temperature inferential control (TIC) is studied for a reactive distillation column with double reactive sections (RDC-DRSs) processing a hypothetical two-stage consecutive reversible reaction ($A + B \rightleftharpoons C + D$, $C + B \rightleftharpoons E + D$ with $\alpha_D > \alpha_B > \alpha_C > \alpha_A > \alpha_E$). Because of the complicated dynamic behaviors, the controlled stages by sensitivity analysis lead to great steady-state deviations (SSDs) in top and bottom product purities. Since TIC involves considerably reduced settling times in comparison with direct composition control, small SSDs in product qualities correspond generally to small transient deviations (TDs) in product qualities. An objective function that measures SSDs in product qualities is formulated to represent the performance of a TIC system and an iterative procedure is devised to search for the best control configuration. The application of the procedure to the RDC-DRS gives considerably suppressed TDs and SSDs in top and bottom product qualities as compared with the one by sensitivity analysis. The method is simpler in principle and less computationally intensive than the current practice. These striking outcomes show the effectiveness of the proposed principle for the development of TIC systems for complicated reactive distillation columns.

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1. Introduction

Temperature inferential control (TIC) is generally advantageous over direct composition control in distillation process operation because temperature sensing needs much less expensive analyzers, lower maintenance costs, and smaller measurement times (*i.e.*, the dead-time introduced to each control loop involved) than composition sensing [1–3]. The former is, however, usually much more difficult to develop than the latter. In addition to the commonly shared problem of pairing controlled variables with manipulated variables, the temperatures of the controlled stages must also be good indications of the product qualities to be controlled and this necessitates an effective determination of the locations of the controlled stages (*e.g.*, the search for the so-called sensitive stages for the rectifying section, reactive section (RS), and stripping section of a reactive distillation column (RDC)). A plenty of criteria and methods have been proposed so far to guide the discrimination process and only have a few of them frequently been employed in the development of TIC systems for various distillation columns, including: (i) slope criterion, (ii) sensitivity criterion, (iii) singular value

decomposition criterion, (iv) invariant temperature criterion, and (v) minimum product variability criterion [4–8]. Although these criteria usually work effectively in the determination of the locations of the controlled stages, they sometimes lead to TIC systems that fail to yield the potentially best control performance especially in the operation of complicated distillation systems through process integration and intensification, *e.g.*, heat-integrated distillation columns, RDCs, and dividing-wall distillation columns [9,10]. This not only limits the applications of TIC systems but also poses negative effect on the development of novel energy efficient distillation systems. Although the determination of the controlled stages appears to be a rather obsolete topic in the area of distillation process control, it has still remained to be an important issue that is worth studying with great attention.

Recently, Kaymak *et al.* studied the operation of a RDC with double reactive sections (RDC-DRS) derived by Yu *et al.*, which processed a hypothetical two-stage consecutive reversible (HTSCR) reaction ($A + B \rightleftharpoons C + D$, $C + B \rightleftharpoons E + D$ with $\alpha_D > \alpha_B > \alpha_C > \alpha_A > \alpha_E$) with a much higher energy efficiency than its conventional counterpart (*i.e.*, a RDC with a single reactive section) [11,12]. Kaymak and his coworkers indicated that the TIC system by sensitivity analysis displayed rather poor performance and was unable to give tight quality control of the top and bottom products. To deal with the difficulty, they devised a composition and temperature combined control system with direct composition control of the top and bottom products and indirect temperature control of the stoichiometric balance between reactants A and B. Although the RDC-DRS could be

[☆] Supported by the National Natural Science Foundation of China (21376018, 21576014, 21676011, 21808007, and 21878011), the Fundamental Research Funds for the Central Universities (ZY1837) and China Postdoctoral Science Foundation (2017M620587).

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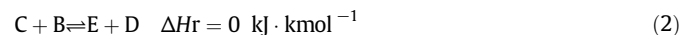
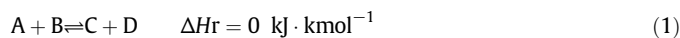
operated smoothly with the composition and temperature combined control system, the involvement of composition measurements degraded definitely, to a certain extent, the control system performance by substantially increasing transient deviations (TDs) and considerably extending settling times. In a more recent paper about the RDC-DRS performing the transesterification of DMC with EtOH to DEC and MeOH, they demonstrated, however, that the TIC system by sensitivity analysis could work effectively to regulate the qualities of the top and bottom products [13]. The completely different outcomes between these two case studies reveal evidently the unique dynamic features of the RDC-DRS. Since the arrangement of multiple reactive sections stands for a much more effective methodology for the development of RDCs, it is imperative to investigate in more detail if the RDC-DRS is likely to be controlled tightly with a TIC system [14–16].

The objective of the current research is to dwell on the TIC of the RDC-DRS separating a reacting mixture involving a HTSCR reaction. Because the TIC system resulted from sensitivity analysis fails to give tight product quality control when facing step changes in product throughput and feed composition, an effective principle and iterative procedure are derived to find the potentially best control configuration that yields the smallest TDs and SSDs in product qualities. Detailed comparisons are made between the resultant TIC systems and the one by sensitivity analysis. After a brief discussion of the obtained outcomes, the article ends with the conclusions that can be drawn.

2. RDC-DRS and its TIC System by Sensitivity Analysis

2.1. Process description

The RDC-DRS studied in this work is sketched in Fig. 1a, which involves totally 30 stages (including condenser and reboiler) [11]. Unlike its conventional analogues, it accommodates the rectifying section, upper RS, middle non-RS, lower RS, and stripping section. The specific structure facilitates the coordination between the reaction operations and separation operation involved and leads consequently to reductions in capital investment and operating cost. While the heavy reactant A is fed onto the top of the upper RS, the light reactant B is divided into two portions with a fixed ratio and introduced, respectively, into the bottom of the upper and lower RS. The top and bottom products are specified to be 95 mol% D and 95 mol% E, respectively. The HTSCR reaction involves five reacting components with the following kinetic and thermodynamic properties.



The reaction rates for the first- and second-stage reactions are

$$R_{1,i} = v_{1,i} H(k_{+1} x_A x_B - k_{-1} x_C x_D) \quad i = A, B, C, \text{ and } D \quad (3a)$$

$$R_{2,i} = v_{2,i} H(k_{+2} x_C x_B - k_{-2} x_E x_D) \quad i = B, C, D, \text{ and } E \quad (3b)$$

where k_{+m} and k_{-m} ($m = 1, 2$) are the rate constants of the forward and backward specific reaction, which can be expressed as

$$k_{+m} = a_{+m} \exp.^{-E+m/RT} \quad m = 1, 2 \quad (4a)$$

$$k_{-m} = a_{-m} \exp.^{-E-m/RT} \quad m = 1, 2 \quad (4b)$$

Table 1 lists the kinetic and physical data of the HTSCR reaction, which are derived in terms of the common characteristics of such kind of reaction systems. Ideal vapor and liquid equilibrium

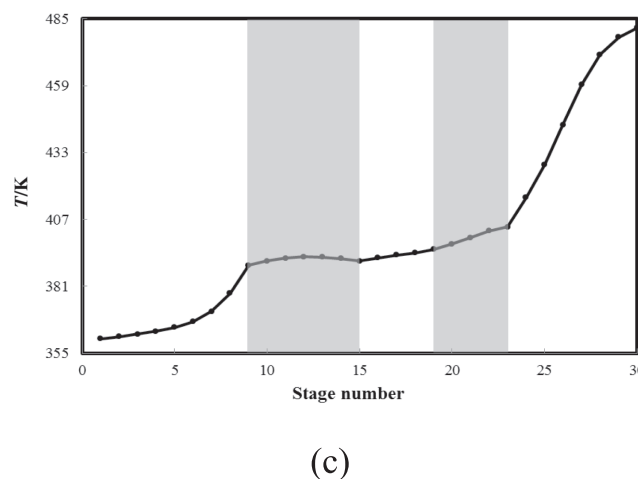
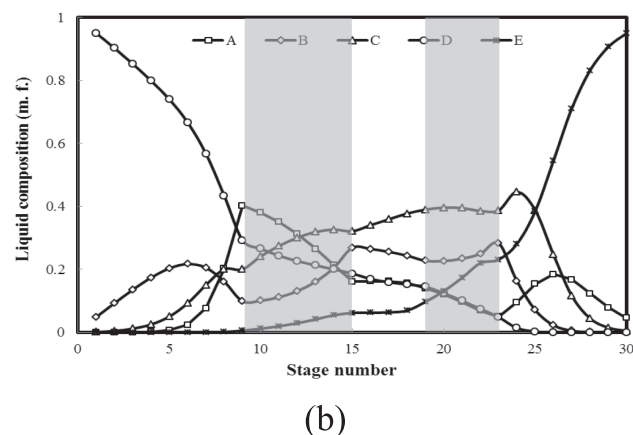
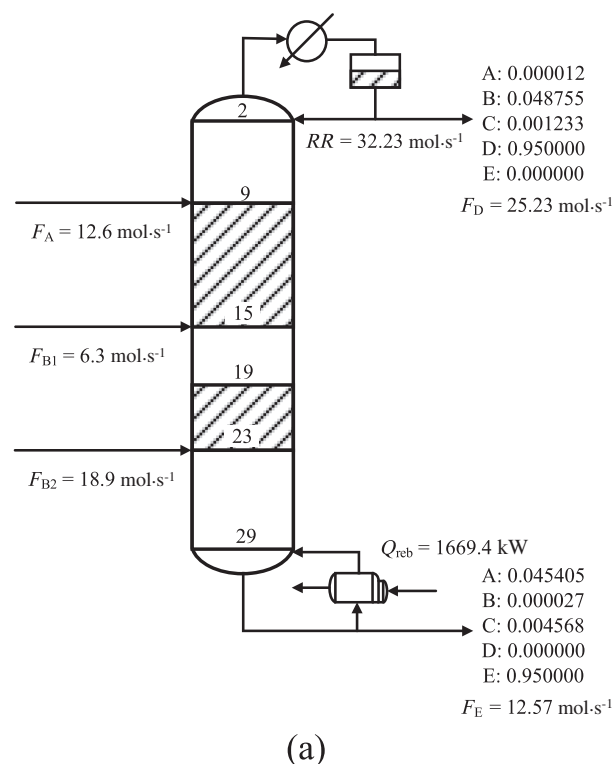


Fig. 1. RDC-DRS and its steady-state behaviors: (a) RDC-DRS; (b) composition profile; (c) temperature profile.

Table 1
Physicochemical characteristics and design specifications of the RDC-DRS (1 cal=4.1868 J)

Parameter	Value
Column pressure/MPa	1
First stage reaction activation energy/kcal·mol ⁻¹	Forward 30 Backward 30
Second stage reaction activation energy/kcal·mol ⁻¹	Forward 30 Backward 30
First stage specific reaction rate at 366 K/kmol·s ⁻¹ ·kmol ⁻¹	Forward 0.008 Backward 0.004
Second stage specific reaction rate at 366 K/kmol·s ⁻¹ ·kmol ⁻¹	Forward 0.0008 Backward 0.0016
First stage chemical equilibrium constant at 366 K	2
Second stage chemical equilibrium constant at 366 K	0.5
Heat of reaction/kcal·mol ⁻¹	0
Heat of vaporization/kcal·mol ⁻¹	6.944
Vapor pressure constants (A _{vp} /B _{vp})	A 10.96/3862 B 12.35/3862 C 11.65/3862 D 13.04/3862 E 10.27/3862

relationships and constant volatilities ($\alpha_D > \alpha_B > \alpha_C > \alpha_A > \alpha_E$) are assumed and the vapor saturation pressure is given by

$$\ln P_i^S = A_{vp,i} - B_{vp,i}/T \quad i = A, B, C, D, \text{ and } E \quad (5)$$

The steady-state and dynamic simulations of the RDC-DRS are carried out in the environment of the commercial software Mathematica. Sketched in Fig. 1b is the steady-state profile of liquid composition. Except that the purifications of products D and E can be clearly seen in the rectifying and stripping sections, it is rather difficult to identify such tendencies in the upper RS, middle non-RS, and lower RS. This phenomenon reflects potentially the strong interactions between the three sections, which may even affect the operation of the rectifying and stripping sections. In terms of the steady-state profile of stage temperatures (c.f. Fig. 1c), a rather flat change is observed in the upper RS, middle non-RS, and lower RS. In spite of the relatively great changes in compositions (for example, components A, D, and E) happen along the three sections, the complicated kinetics of the HTSCR reaction suppresses substantially the changes in temperature and consequently results in the intensive coupling between the three sections.

2.2. TIC system by sensitivity analysis

Instead of the three-point temperature control configuration examined by Kaymak *et al.*, a more complicated one that involves four temperature control loops is adopted here in the current work. System pressure is maintained at 1 MPa with the manipulation of heat removal from condenser. The reflux drum level is controlled with the flow rate of top product and the reboiler level with the flow rate of bottom product. The fresh feed flow rate of reactant A (F_A) is flow controlled and serves as the production rate handle. The two fresh feed flow rates of reactant B, F_{B1} and F_{B2} , are paired with the temperatures of two stages to be selected, serving to maintain the stoichiometric balance with reactant A. The reflux flow rate, RR , and reboiler heat duty, Q_{reb} , are used to control the temperatures of two stages to be selected, working, respectively, to maintain the purity of component D in the top product and the purity of component E in the bottom product.

In Fig. 2 are given the results of sensitivity analysis for the RDC-DRS. Here, sensitivity serves to measure the variability of stage temperatures to a change in one of the four manipulated variables (i.e., F_{B1} , F_{B2} , RR , and Q_{reb}). Note that the RDC-DRS displays sharply different behaviors from conventional distillation columns. In the case of an increase in reboiler duty, the conversion rate goes down and results in the increase in the composition of component A and the

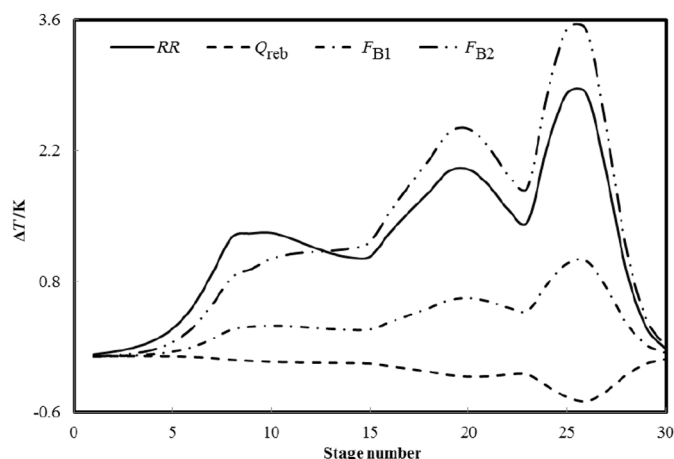


Fig. 2. Sensitivity analysis of the RDC-DRS.

decrease in the composition of component E in the upper and lower parts of the RDC-DRS, respectively. Thus, the temperature drops along the whole column. In the case of an increase in the feed flow rate of reactants A and B and the reflux flow rate, the conversion rate goes up and results in the increase in the composition of component E along the whole column. Thus, the stage temperature shows unexceptionally an increase in these cases. Q_{reb} exhibits only a negative peak on stage 26 where RR , F_{B1} , and F_{B2} show, respectively, their highest peaks. While the latter three variables present, respectively, their second peaks on stage 20, RR and F_{B1} display their third peaks on stage 10. The common positions of the peaks reveal the potentially intensive coupling between the controlled variables to be chosen. In accordance with the relative gain array (RGA) listed in Table S1 of the supplementary information and the proximity principle, while RR should be paired with T_{10} , Q_{reb} should be with T_{26} and F_{B1} and F_{B2} should, respectively, be with T_{20} and T_{24} (it is chosen from the stages near F_{B2}). The resultant control configuration is sketched in Fig. 3a and labeled the CS1, hereinafter. P controllers (with a gain of 2) are applied to the two liquid level control loops and PI controllers are for the four temperature control loops. Two 60s first-order measurement lags are included in each temperature measurement. All temperature controllers are tuned with the Tyreus-Luyben rule and the obtained parameters are listed in Table 2. Because the open-loop gain of the bottom control loop is considerably smaller than those of the other control loops, a much larger K_c value is required in this control loop than in the other control loops. This outcome also reflects the unique characteristics of the RDC-DRS.

The closed-loop responses (CLRs) of the CS1 to a $\pm 20\%$ step change in production rate handle are illustrated in Fig. 4. Throughout the article, unless otherwise stated, the positive responses are represented by black curves and negative responses by gray curves. The F_{B1} and F_{B2} control loops fail to work effectively to keep the stoichiometric balance between reactants A and B and force the top and bottom products to exhibit rather great peak deviations. Although stable operation is secured, the top and bottom products converge finally to new steady-state values (SSVs) and cannot be recovered back to their set-points. Table 3 lists their absolute and relative SSDs. While in the case of the $+20\%$ throughput change, the D composition in the top product and E composition in the bottom product stabilize at 0.9417 and 0.952, respectively, in the case of the -20% throughput change, they level out at 0.958 and 0.9474, respectively. Given in Fig. 5 are the CLRs of the CS1 to a $+5\%$ step change of B composition in F_A . In addition to the rather great peak deviations in the top and bottom products, they converge to new SSVs and cannot be recovered back to their set-points. Table 3 also includes their absolute and relative SSDs. The D composition in the top

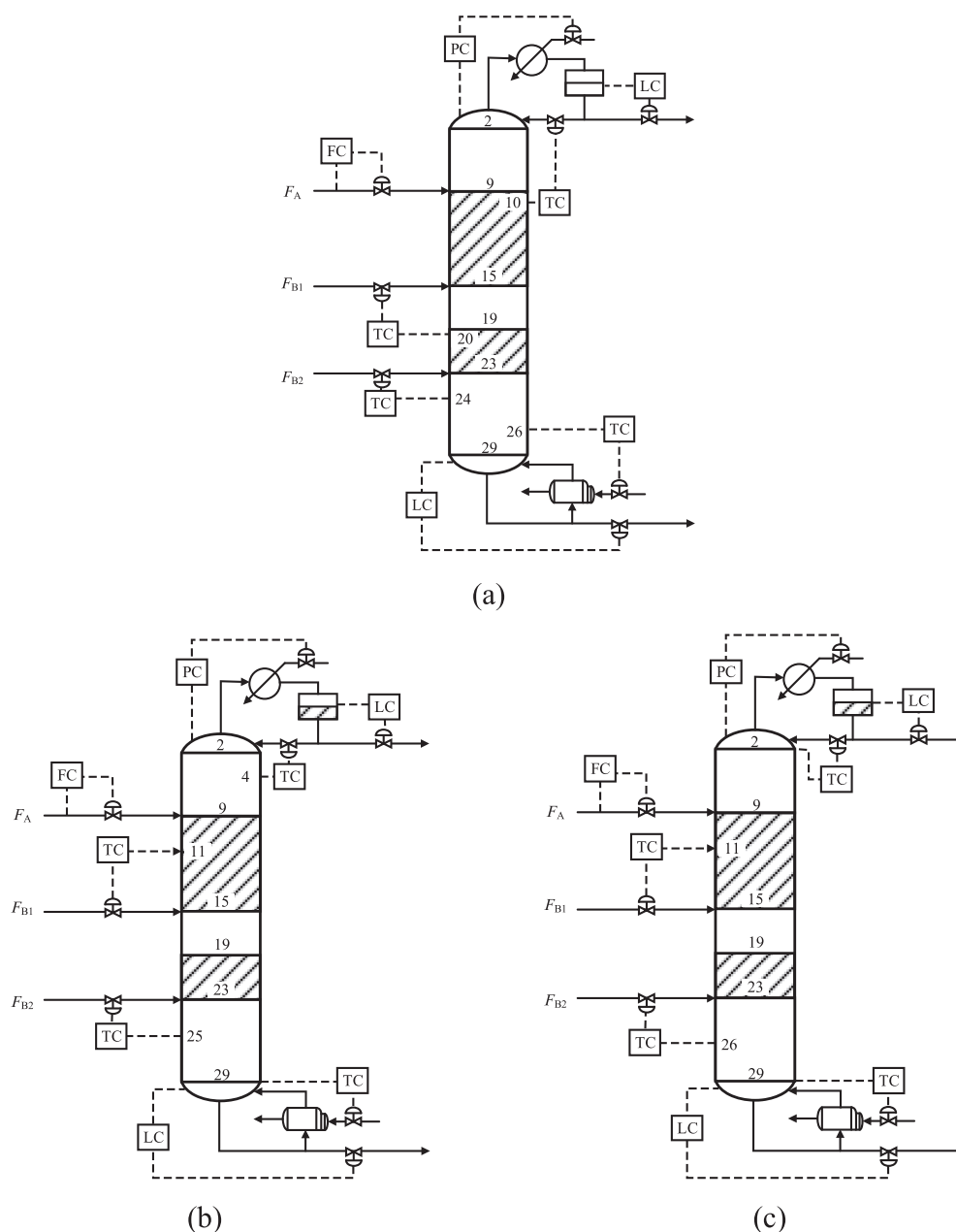


Fig. 3. TIC schemes of the RDC-DRS: (a) CS1; (b) CS2; (c) CS3.

product and E composition in the bottom product stabilize at 0.9398 and 0.9496, respectively. The F_{B1} and F_{B2} control loops fail again to work effectively in maintaining the reactant A and B's stoichiometric

Table 2
Controller parameters of the CS1, CS2, and CS3

Control scheme	Control loop	K_C	T_i/min
CS1	Top	2	12
	F_{B1}	2.75	12.8
	F_{B2}	5	4.4
	Bottom	5×10^4	4.5
CS2	Top	8	3.6
	F_{B1}	1.25	98.4
	F_{B2}	3	4.5
	Bottom	1×10^6	1.2
CS3	Top	250	0.1
	F_{B1}	1.45	34.8
	F_{B2}	3	4.5
	Bottom	1×10^6	1.2

balance and result in an excess of reactant B. The excess of reactant B initiates further a transition to a new steady state and this can clearly be identified from the response of the top control loop. Around the instant of 0.667 h, the D composition in the top product already reaches the vicinity of an intermediate steady state. Despite that the four manipulated variables (i.e., F_{B1} , F_{B2} , RR , and Q_{reb}) have involved no sharp changes since that time instant, the D composition in the top product fails to settle down to that intermediate steady state. Instead, it still displays a long excursion with a very different speed from the one before that time instant. This outcome implies that the CS1 cannot effectively deal with the output multiplicity of the RDC-DRS.

It seems that the TIC system by sensitivity analysis cannot hold tight operation of the RDC-DRS. The reason should definitely be attributed to the strong coupling between the controlled stages chosen. To deal with the failure, one has to ascertain if alternative controlled stages can be found that is likely to result in alleviated interaction between the four control loops. Thus, an effective principle and procedure should be developed for that purpose.

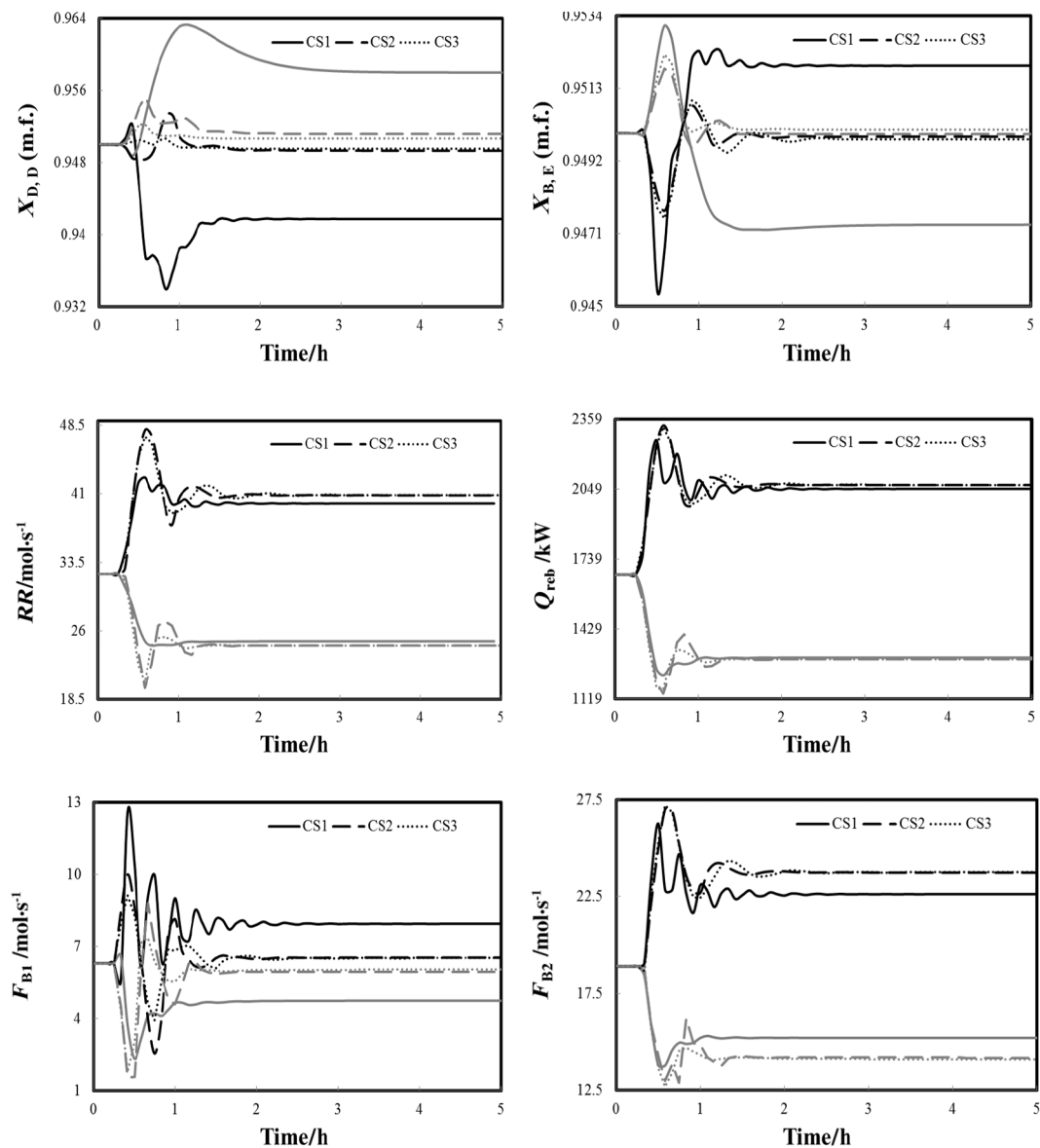


Fig. 4. Comparison between the CS1, CS2, and CS3 schemes in face of a $\pm 20\%$ step change in F_A .

3. A Novel Principle and Procedure for the Development of a TIC System

3.1. A novel principle for the development of TIC system

Generally speaking, the performance of a TIC system should be evaluated in terms of both TDs and SSDs in product qualities. Because

temperatures are dominant variables in a distillation column, their tight control leads generally to considerably reduced settling times as compared with direct composition control [17]. Moreover, the settling times are generally not so sensitive to the changes in the locations of the controlled stages. Such characteristics might allow the small SSDs in product qualities correspond generally to the small TDs in product qualities. It seems therefore reasonable to evaluate the

Table 3
SSDs of the CS1, CS2, and CS3

Scenario	Deviation	CS1		CS2		CS3	
		Absolute error	Relative error	Absolute error	Relative error	Absolute error	Relative error
+ 20% in F_A	$ \Delta X_{D,D} $	8.256×10^{-3}	0.869%	6.930×10^{-4}	0.073%	4.770×10^{-4}	0.050%
	$ \Delta X_{B,E} $	1.953×10^{-3}	0.206%	9.500×10^{-5}	0.010%	1.700×10^{-4}	0.018%
− 20% in F_A	$ \Delta X_{D,D} $	7.978×10^{-3}	0.840%	1.156×10^{-3}	0.122%	6.653×10^{-4}	0.069%
	$ \Delta X_{B,E} $	2.643×10^{-3}	0.278%	1.600×10^{-5}	0.002%	1.150×10^{-4}	0.012%
5% B in F_A	$ \Delta X_{D,D} $	1.024×10^{-2}	1.078%	1.151×10^{-3}	0.121%	4.320×10^{-4}	0.045%
	$ \Delta X_{B,E} $	4.030×10^{-4}	0.042%	4.240×10^{-4}	0.045%	3.010×10^{-4}	0.032%
	J_k	3.147×10^{-2}	100%	3.535×10^{-3}	11.232%	2.148×10^{-3}	6.824%

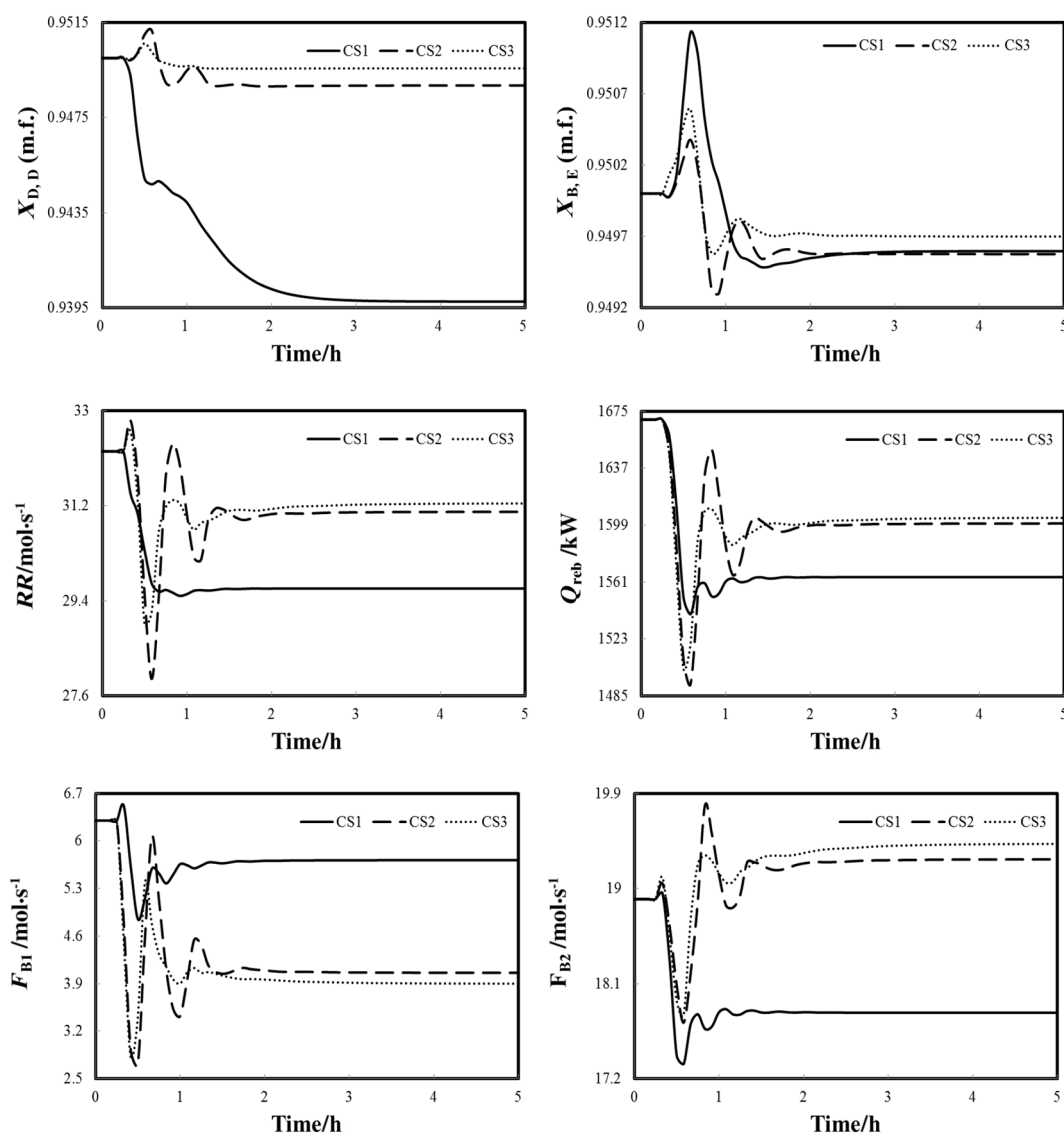


Fig. 5. Comparison between the CS1, CS2, and CS3 schemes in face of a 5% step change of B composition in F_A .

performance of a TIC system in terms of merely SSDs in product qualities. The simplification of the evaluation metric can greatly facilitate the determination of the controlled stages since the search process is now turned from a dynamic optimization to a static one with the steady-state model as an equality constraint. Hori and Skogestad once employed a kind of metric describing the SSDs in product qualities to locate the appropriate controlled stages for two-product distillation columns [18]. With reference to the RDC-DRS, the following sum of the absolute SSDs caused by the step changes in feed flow rates and compositions can be constructed as the objective function for the search of the best controlled stages.

$$J(L1, L2, L3, L4) = \sum_i (|\Delta X_{D,i}| + |\Delta X_{B,i}|) \quad (6)$$

$i = \pm 20\%$ changes of F_A and 5% change of B composition in F_A

where L1, L2, L3, and L4 are the controlled stages' locations in the RR , F_{B1} , F_{B2} , and Q_{reb} control loops.

The objective function of Eq. (6) equally treats the disturbances from feed flow rates and compositions and so do the SSDs in the top and bottom products. If necessary, weighting coefficients can be included to represent their relative impacts on control system performance.

3.2. An iterative procedure for the development of TIC system

Because the formulation of Eq. (6) is essentially a mixed integer non-linear optimization problem and its solution is rather complicated in principle and fairly time-consuming in search computation. To avoid the drawbacks, we develop an iterative procedure as given in Fig. 6 for the determination of controlled stages with the application of a uni-variable search method reinforced with some heuristic evolutionary principles. The initial controlled stages are determined with a conventional criterion (e.g., the sensitivity analysis here) followed by pairing them with the available manipulated variables. If the resultant control system performance appears satisfactory in terms of the SSDs in product qualities, then the tuning of the temperature controllers can proceed; otherwise, the loop-by-loop adjustment of the controlled stages should be performed. During the process, the location of the controlled stage for each control loop is adjusted until the objective function of Eq. (6) has reached its minimum value. The search process stops in case that there is only negligible changes in the objective function of Eq. (6) between the two adjacent rounds of iterations. Because of the possibly drastic changes in the locations of the controlled stages, their pairing with the available manipulated variables should again be examined here. It should be indicated that the proposed iterative procedure is much more effective than the ordinary sequential enumeration method.

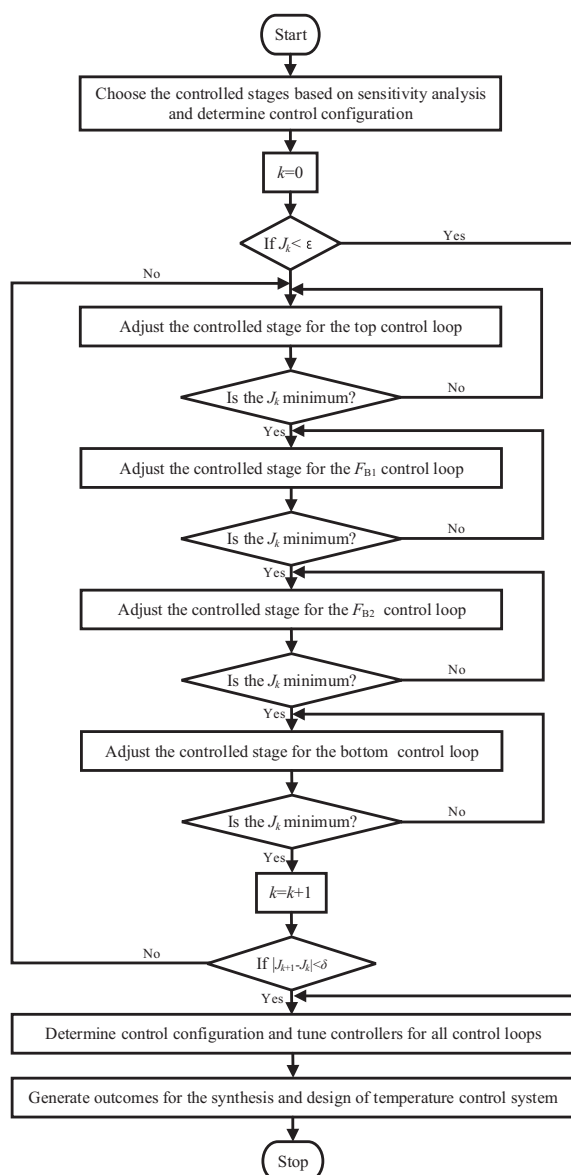


Fig. 6. An iterative procedure for the synthesis and design of a TIC system for the RDC-DRS.

Although the optimality cannot theoretically be guaranteed with the adopted uni-variable search method, it can, in most cases, lead to reasonable approximate solution to the formulation of Eq. (6).

4. Development of a TIC System for the RDC-DRS

The RDC-DRS' steady-state model described in the supplement information is employed in the current study. With the application of the iterative procedure shown in Fig. 6 to the RDC-DRS, the obtained relationships between the objective function of Eq. (6) and the locations of the controlled stages are displayed in Fig. 7 for the first round of iterations ($k = 1$). Due to the effective use of the knowledge gained from the intermediate search processes, only 8 times of steady-state model calculations are actually required. In the top control loop (c.f. Fig. 7a), the objective function decreases steadily by moving the controlled stages from stage 10 to stage 4. Further ascending the controlled stage causes no convergence in steady-state simulation and this signifies that the temperatures on the chosen stages cannot be kept constant in face of disturbances from feed flow rates and compositions. Thus the adjustment should end up at stage 4. In the F_{B1} control loop (c.f. Fig. 7b), the objective function decreases steadily by moving the

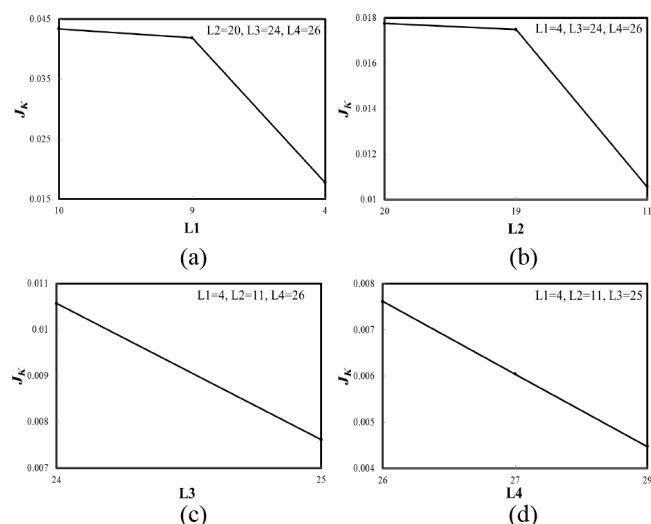


Fig. 7. Objective function versus the controlled stages ($k = 1$): (a) top control loop; (b) F_{B1} control loop; (c) F_{B2} control loop; (d) bottom control loop.

controlled stages from stage 20 to stage 11. Further ascending the controlled stage causes no convergence in steady-state simulation and thus the adjustment ends up at stage 11. In the F_{B2} control loop (c.f. Fig. 7c), the objective function decreases steadily by moving the controlled stages from stage 24 to stage 25. For the avoidance of the same controlled stage with the bottom control loop, the adjustment ceases to stage 25. In the bottom control loop (c.f. Fig. 7d), the objective function decreases steadily by moving the controlled stages from stage 26 to stage 29. The first round of iterations ($k = 1$) leads to a substantial reduction of the objective function and gives rise to the control configuration as sketched in Fig. 3b and labeled the CS2, hereinafter.

Fig. 8 illustrated the obtained relationships between the objective function of Eq. (6) and the locations of the controlled stages for the second round of iterations ($k = 2$). Here only 5 times of steady-state model calculations are needed. In the top control loop (c.f. Fig. 8a), the objective function decreases again by moving the controlled stages from stage 4 to stage 2 and no divergence problems occur any more in these cases. In the F_{B2} control loop (c.f. Fig. 8c), the objective function exhibits its minimum value at stage 26. In the other two control loops (c.f. Fig. 8b and d), the current controlled stages keep, respectively, the

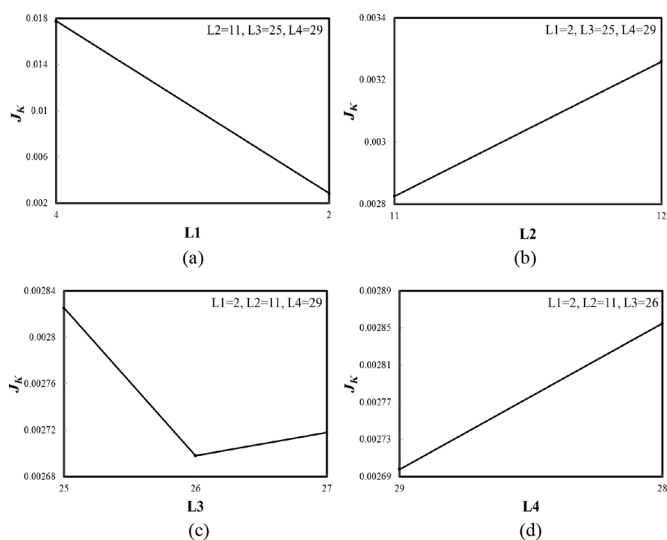


Fig. 8. Objective function versus the controlled stages ($k = 2$): (a) top control loop; (b) F_{B1} control loop; (c) F_{B2} control loop; (d) bottom control loop.

objective function at its minimum value and thus no adjustments are needed any more. The second round of iterations ($k = 2$) leads again to a substantial reduction of the objective function and gives rise to the control configuration as sketched in Fig. 3c and labeled the CS3, hereinafter. The third round of iterations ($k = 3$) is conducted and no adjustment of the controlled stages are necessary. Note the fact that the CS3 conforms well to the proximity principle and the prediction by the RGA listed in Table S2 of the supplementary information.

Also given in Fig. 4 are the CLRs of the CS2 and CS3 to a $\pm 20\%$ step change in the production rate handle. It is noted that the peak deviations are suppressed substantially in the top and bottom products with almost the same settling times with the CS1. Although new SSVs are reached, the SSDs are substantially suppressed and the detailed outcomes are also summarized in Table 3. While for the positive change, the CS2 reduces the SSDs in the top and bottom products by 0.796% and 0.196%, respectively, in comparison with the CS1, for the negative change, the two numbers become 0.718% and 0.276%, respectively. In comparison with the CS2, while the CS3 reduces the SSD of the top product by 0.023% and increases the SSD of the bottom product by 0.008%, for the positive change, for the negative change, the CS3 reduces the SSD in the top product by 0.053% and increases the SSD of the bottom product by 0.01%. In other words, a more coordinated system performance is reached by the CS3 than by the CS2 between the RR and Q_{reb} control loops.

Also given in Fig. 5 are the CLRs of the CS2 and CS3 to a 5% step change of B composition in F_A . Again, the peak deviations are suppressed substantially in the top and bottom products. They still settle down into new SSVs, but their SSDs are again substantially suppressed in these situations. In comparison with the CS1, the CS2 reduces the SSD of the top product by 0.957% and increases the SSD of the bottom product by 0.003%. In comparison with the CS2, the CS3 reduces the SSD of the top and bottom products by 0.076% and 0.013%, respectively. Again, a more coordinated control performance is reached by the CS3 than by the CS2 between the RR and Q_{reb} control loops. The detailed outcomes can also be identified from Table 3.

With reference to the objective function, the CS2 and CS3 abate, respectively, its value by 88.768% and 93.176% as compared with the CS1, implying evidently a monotonic improvement in control system performance by the iterative procedure shown in Fig. 6.

5. Discussions

The failure of the TIC system (resulted from sensitivity analysis) in securing tight product quality control is certainly aroused by the complicated dynamic behaviors of the RDC-DRS, *i.e.*, the inherent strong interaction and the high degree of process nonlinearity. With the application of the novel principle and procedure proposed in the current work, the drawbacks of the TIC system are gradually alleviated and the potentially best TIC system can be approached, which gives rise to considerably suppressed TDs and SSDs in the top and bottom product qualities. It is noticed that even in the presence of output multiplicities (note that the very different SSVs of F_{B1} and F_{B2} between the CS1, CS2 and CS3 also give support to the transition to a new steady state of the RDC-DRS incorporated with the CS1), the proposed novel principle and procedure can still work effectively. These outcomes demonstrate definitely their rational and effectiveness. Since merely SSDs in product qualities are involved in the objective function of Eq. (6), the derivation of control configuration and the tuning of controllers can be executed in a sequential manner and this facilitates the search process to be not only simpler in principle but also less computationally intensive than the current practice.

To further evaluate the feasibility and effectiveness of the proposed principle and procedure for the development of the TIC for the RDC-DRS, we also examine here the influences of different control loop search sequences and different pairings between the manipulated and controlled variables and the detailed outcomes are included in the

Supporting Information. In terms of a sharply different control loop search sequence, L2, L3, L4, and L1, the obtained relationships between the objective function of Eq. (6) and the locations of the controlled stages are included in Figs. S1 and S2 of the supplementary information for the first and second rounds of iterations. With totally 13 times of steady-state model calculations, the CS3 is reached. In terms of a sharply different pairings between the manipulated and controlled variables, $RR-T_{26}$, $F_{B1}-T_{24}$, $F_{B2}-T_{20}$, and $Q_{reb}-T_{10}$, the obtained relationships between the objective function of Eq. (6) and the locations of the controlled stages are depicted in Figs. S3 and S4 of the supplementary information for the first and second rounds of iterations. With totally 14 times of steady-state model calculations, the CS3 is also reached. In terms of a sharply different control loop search sequences L2, L3, L4, and L1 and sharply different pairings between the manipulated and controlled variables, $RR-T_{26}$, $F_{B1}-T_{24}$, $F_{B2}-T_{20}$, and $Q_{reb}-T_{10}$, the obtained relationships between the objective function of Eq. (6) and the locations of the controlled stages are delineated in Figs. S5 and S6 of the supplementary information for the first and second rounds of iterations. With totally 13 times of steady-state model calculations, the CS3 can again be reached. In spite of the sharply different control loop search sequences and different pairings between the manipulated and controlled variables, the three situations converge unexceptionally to the outcome of Figs. 7 and 8 with somewhat similar computational requirement. These outcomes indicate that the proposed principle and procedure can work effectively for the development of TIC systems for the RDC-DRS separating the HTSCR reaction.

6. Conclusions

The complicated dynamics of the RDC-DRS preclude the TIC system resulted from sensitivity analysis to achieve tight product quality control. This observation, however, does not necessarily signify that TIC is inapplicable and ineffective in this situation. In fact, through the deliberate discrimination of controlled stages in the development of the TIC system, its performance can, in most cases, be substantially enhanced and tight product quality control is likely to be achieved. Because the changes in controlled stages usually do not influence very much the settling times of a TIC system, an objective function that measures merely the SSDs in product qualities can frequently be formulated to describe the dynamic performance of the TIC system. An iterative procedure has been devised to search for the potentially best control configuration that gives rise to the smallest TDs and SSDs in product qualities. Through the comparison with the one by sensitivity analysis, the resultant TIC system suppresses considerably the SSDs in product qualities and can be used to secure tight control of the RDC-DRS. Since no prerequisites at all are needed on the steady-state and dynamic characteristics of the process to be controlled, the proposed novel principle and procedure are deemed to be applicable to any other types of complicated RDCs.

Supplementary Material

Supplementary material to this article can be found online at <https://doi.org/10.1016/j.cjche.2018.11.023>.

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