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Dynamic Controllability Investigation of an Energy-Saving Double Side-Stream Ternary Extractive Distillation Process

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Abstract: The investigation of dynamic controllability for the double side-streams ternary extractive distillation (DSTED) is necessary due to its advantages in energy-efficient. However, the control strategy of the energy-saving DSTED scheme is unique and complex issues owing to the wobbly of side-stream flow rate. Herein, control strategy of the energy-saving DSTED scheme is explored for separating ternary azeotropic mixtures acetonitrile/methanol/benzene. Inspiring from the control strategy of the ordinary triple-column extractive distillation scheme, the fundamental control structure CS1 is firstly designed. The control scheme CS2 with feed/side-stream (F/SS) ratio and control structure CS3 with feedforward and F/SS are then investigated to achieve higher efficiency of process control. Finally, a robust control strategy CS4 with the ratio of reboiler duty and feed flow rate and without F/SS ratio is proposed to well maintain the product purities. Moreover, additional ±15% feed flow rate and composition disturbances are added in the CS4 to assess the stability and controllability of the energy-saving DSTED. Dynamic performances illustrate that the structure CS4 can handle as well as that of confronted ±10% disturbances when the large disturbances are occurred in the real chemical process.

Keywords: ternary azeotropic mixtures; dynamic control; separation; side-stream extractive distillation

1. Introduction

As is well-known, the separation of mixtures by heating the mixtures of liquid to balanced state based on differences in the relative volatility or boiling point of components is called as distillation process [1]. It is the usually commonly employed separation technique because of its superiority in the operation and control for the chemical engineering processes [2]. However, the mixtures of production in the industry are always non-ideal azeotropic system [3]. As a consequence, some special separation techniques (such as pressure-swing [4-8], azeotropic [9, 10] and extractive distillations [11-17]) are proposed to separate such azeotropic non-ideal systems.

Extractive distillation (ED) is the most commonly technique for the separation of close-boiling point (relative volatility is close to 1) or azeotropic mixtures (relative volatility of an azeotropic point is 1). Although the ED technique is always applied, one major obstacle is required a lot of energy (i.e., steam) to achieve the separation task. Hence, a lot of researches on energy-efficient investigation of ED (e.g., pressure-swing, heat integration and side-stream) are presented and much has been achieved so far. For instances, Gu et al. [18] presented a novel concept to obtain the optimal extractive distillation with a heat integration under a suitable low pressure for separating minimum-azeotropic mixtures tetrahydrofuran/water using entrainer dimethyl sulfoxide and they illustrated that total annual cost of the proposed configuration is reduced by 20.3% than the existing design. You et al. [19] investigated a novel energy-saving extractive distillation process to separate azeotropic mixtures acetone/methanol by varying the pressure and they proved that total heat duty and annual cost of the proposed scheme are reduced 33.9% and 30.1%. Extractive dividing wall column (EDWC) for separating the methylal/methanol binary azeotropic mixtures with dimethylfomamide as an entrainer is reported by Xia et al. [20], and they demonstrated that the intensified scheme can save 11.60% of total annual cost. Yang et al. [21] proposed a heat integration

EDWC with an additional decanter process for separating ternary heterogeneous mixtures methanol/toluene/water and they proved that the total annual cost of the proposed process have 15.14% reduction reduced compared with the heat integrated double-column process. A significant investigation for the application of the EDWC scheme to separate benzene/cyclohexane system is proposed by Sun et al. [22] and they demonstrated that the TAC of 4.8% could be saved via the proposed EDWC scheme. Tututi-Avila et al. [23] found the EDWC for separating the azeotrope mixture ethanol/water causing 12.42% reduction in the total annual cost than the two columns extractive distillation process. Chien's group reported a 1.79% reduction in total annual cost in the separation of binary system acetone/methanol using the improved EWDC sequence compared with the existing extractive distillation [24]. In summary, the proposed intensification technologies can effectively reduce the energy consumption of the process, but it makes the operability and control of the proposed process become more complicated and tougher than conventional process. Hence, it is profound significance to present a robust control scheme for energy-efficient extractive distillation techniques.

Dynamic performances of energy-efficient extractive distillation techniques have been also investigated substantially in the literature. For example, Luyben [25] explored the dynamic controllability of the low solvent-to-feed ratio (S/F) ED sequence. The calculations demonstrated that performances of the nonlinear S/F control strategy could be effectively improved than the existing structure of the ED scheme. The dynamic investigation of the pressure-swing double-column extractive distillation confronting disturbances in feed flow rates and composition is reported by Li et al. [26] and the dynamic responses illustrated that the recycled stream should be determined as a key controlled variable to maintain purity of product. Wu et al. [27] investigated that two products in the EDWC can still be controlled at high purity by using a simple temperature control scheme to manipulate reboiler duties. An improved control structure with the ratio of reboiler duty and feed (Q_R/F) is established by Xia et al. [20] and they proved that the product purity could be well controlled with a small response time and offsets via an effective composition/vapor split ratio cascade control strategy. Recently, our research group [21] proposes a robust control structure with temperature-feed/solvent cascade, and the results demonstrated that three product purities can be well maintained at specified purity.

Recently, several energy-saving schemes (e.g., dividing wall column, side-stream, and hybrid process) have been investigated by Wang et al. [28] and they illustrated that the double side-streams ternary extractive distillation column (DSTED) to separate ternary azeotropic system acetonitrile, methanol and benzene using solvent chlorobenzene is most promising among those energy-effective processes from the economic aspect. Following that, a composition control structure strategy is explored to handle three product purities [12]. However, a composition controller should be avoided because of it is not recommended in industrial processes [29]. Therefore, to ensure the production purity and stable operation, more attention should be focused on to develop a simple and effective temperature control strategy for DSTED process when handling feed compositions and feed flow rates disturbance.

The contribution of this work is to investigate the dynamic controllability of the energy-saving DSTED process via an inexpensive temperature control scheme. The basic control structure of the energy-saving process for separating mixtures acetonitrile/methanol/benzene is first designed based on the conventional triple-column extractive distillation process. The key factors of side-stream are studied to reduce the peak transient deviations and offsets of control structures. Furthermore, two robust feedforward control strategies for this energy-saving process are investigated to reduce the time of reach steady state and instantaneous vibration when confronting with feed flow rate and composition disturbances. To evaluate the stability and robustness of the proposed control strategies, the ±10% and ±15% feed flow rates and compositions disturbances are introduced.

2. Steady-State Simulation

Herein, the detailed steady-state design parameters of the DSTED for separating acetonitrile/methanol/benzene are obtained from the work of Wang et al. [28]. The flowsheet of the DSTED with detailed information is displayed in Fig. 1.

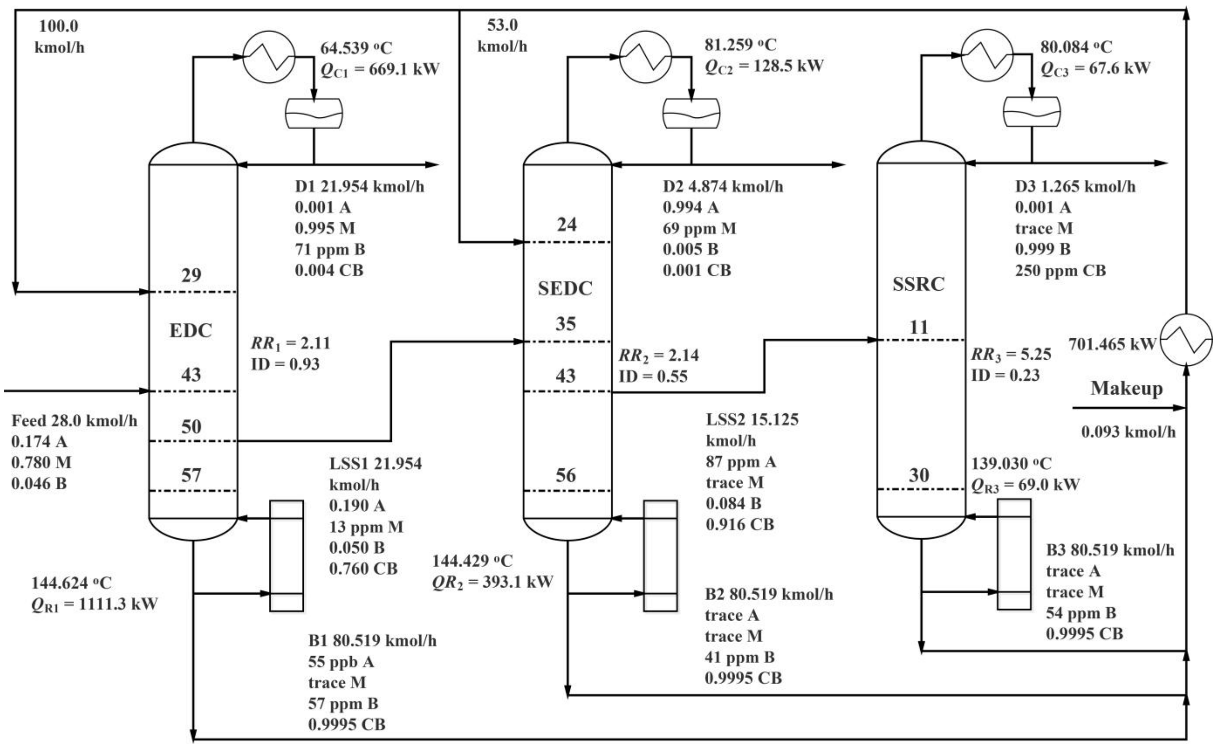

Fig. 1. Flowsheet of the energy-saving DSTED for separating acetonitrile/methanol/benzene

The fresh feed flowrates of ternary mixtures are 28 kmol/h with composition 17.4 mol% acetonitrile, 78.0 mol% methanol and 4.6 mol% benzene. Extractive distillation column, side extractive distillation column, and side solvent recovery column are represented as EDC, SEDC, and SSDC, respectively. Vapor-liquid equilibrium of this ternary azeotropic system using chlorobenzene as solvent [28] could be well described via the Wilson model. The reproduced results are slightly different from the study of Wang et al. [28]. Of note is that, the purity of acetonitrile is lower and the purity of benzene is higher than Wang's work because of the inaccurate reflux ratio with three significant digits and different convergence methods are used in this work. However, this will not affect the control design of DSTED process. Before implementing to the Aspen dynamic mode, the main parameter is set to below [2, 3]:

(1) Tray pressure drops in three columns are set to 0.7 kPa;
(2) 5 min of residence time are used to calculate the liquid holdups in reflux drums and sumps when they reach a half-full;
(3) Pressure drop of 2 bar is given in all valves.

3. Dynamic Control for the DSTED

3.1 Determination of temperature control trays

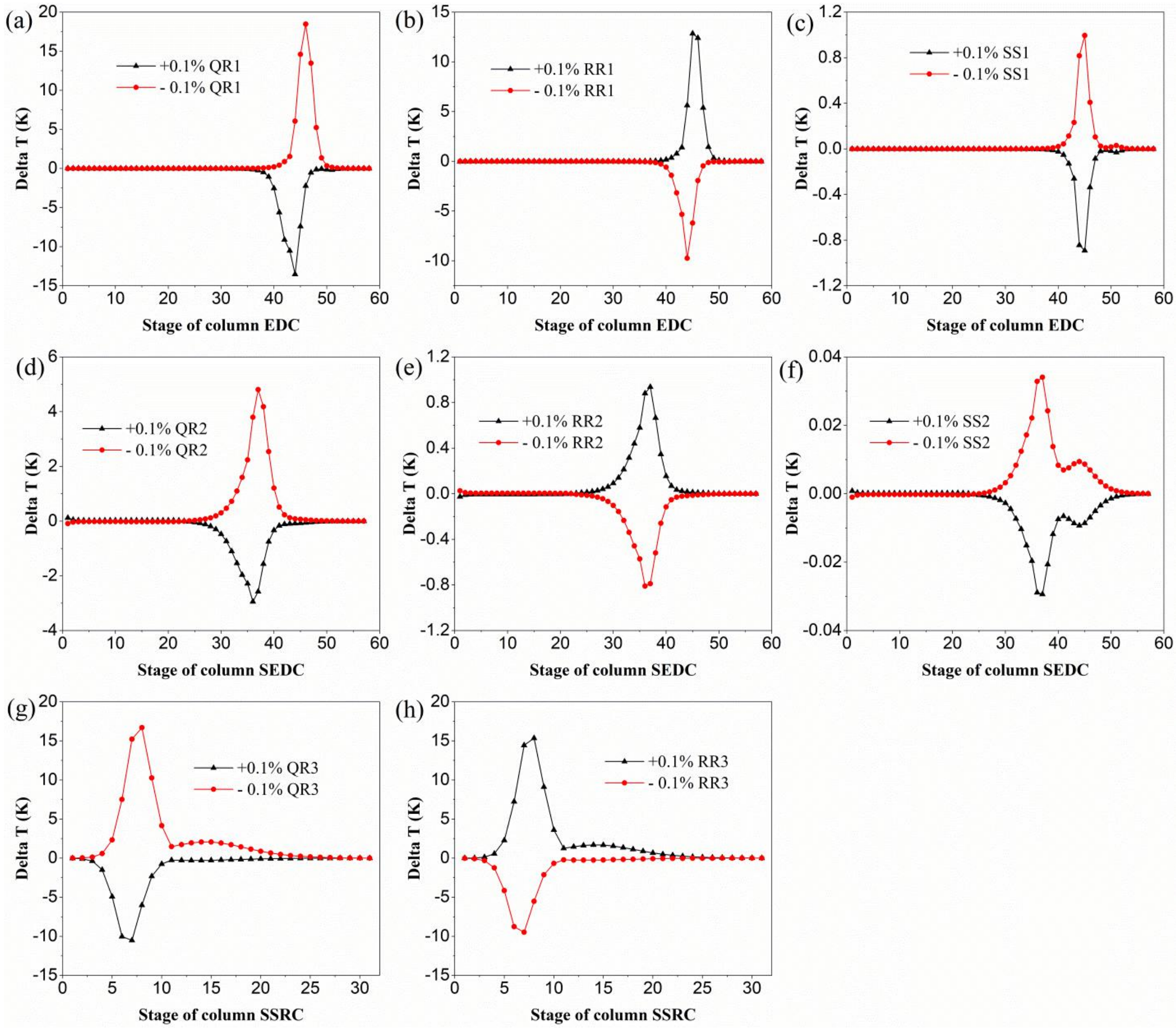

Fig. 2. Open-loop sensitivity analysis by varying manipulated variables

The temperature control points need to be firstly determined. Temperature-sensitive trays of three columns are selected via the open-loop sensitivity analysis [15, 30] as shown in Fig. 2. Temperatures of 45th, 36th and 7th stages have large peaks indicating that these stages can be determined as temperature-sensitive stages to maintain product purities.

3.2 Basic control structure CS1

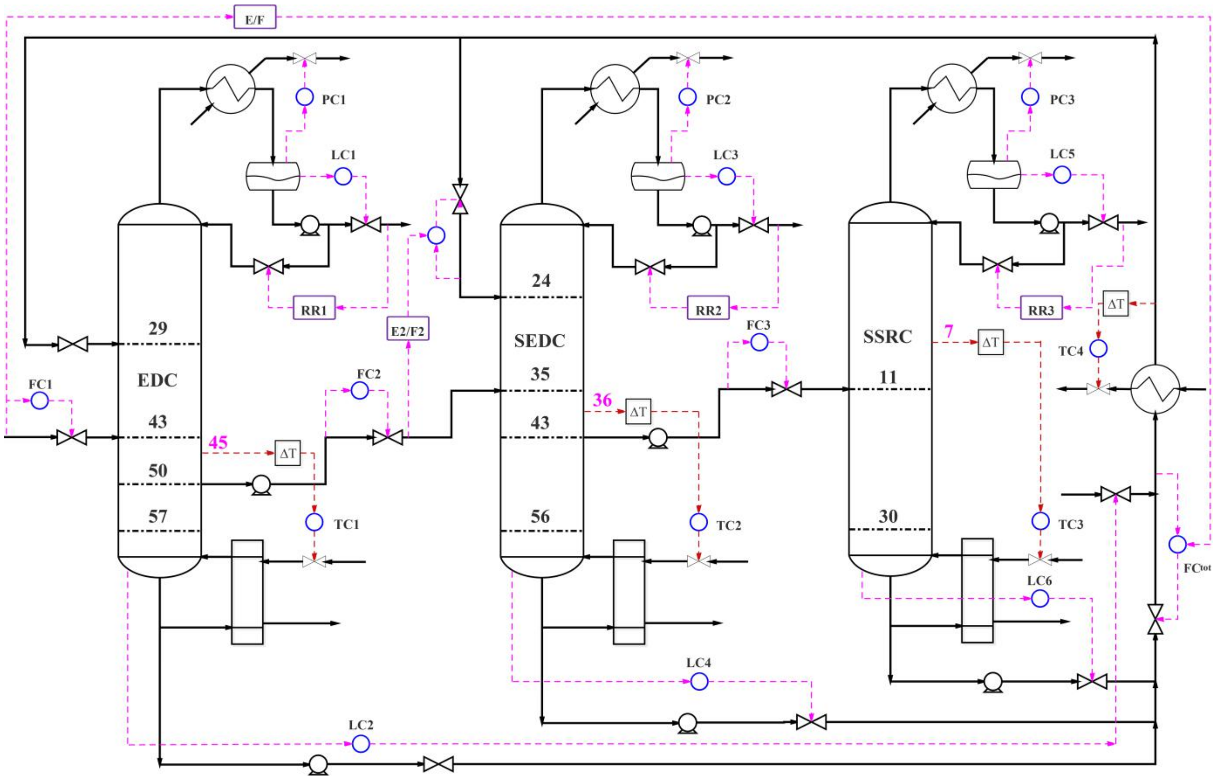

Fig. 3. Basic control structure CS1 for DSTED system

Fig. 3 illustrates the basic control scheme of the DSTED process is explored based on the control scheme of the triple-column extractive distillation sequence for the separation of ternary mixture of tetrahydrofuran/ethanol/water [31] and ethyl acetate/ethanol/water [15].

Gain K_C = 2 and a large integral time τ_I = 9999 min are given in all level controllers (i.e. LC1, LC2, LC3, LC4, LC5 and LC6) [2]. K_C and τ_I of all pressure controllers (i.e. PC1, PC2 and PC3) are set to default values 20 and 12, respectively [3]. K_C of 0.5 and τ_I of 0.3 min of feed controllers (i.e. FC1, FC2, FC3 and FC_{tot}) settings are suggested by Yang et al. [21]. In addition, dead time with

2 min is inserted to the four temperature control loops (i.e. TC1, TC2, TC3 and TC4) [32-35]. According to Luyben [36], Tyreus–Luyben method (see in Eqs. 1–2) are used to tune the temperature controllers of column and heat exchanger. Finally, the K_C and τ_I is obtained via relay-feedback and summarized in Table 1.

$$K_C = K_U / 3.2 \quad (1)$$

$$\tau_I = 2.2P_U \quad (2)$$

Table 1. Tuning parameters of CS1 for the DSTED process

	TC1	TC2	TC3	TC4
Ultimate gain, Ku	1.4445	2.3225	1.3337	0.5215
Ultimate period, Pu (min)	9.6000	13.8000	9.6000	3.6000
Gain, K_C	0.4514	0.7258	0.4168	0.1630
Integral time, τ_I (min)	21.1200	30.3600	21.1200	7.9200

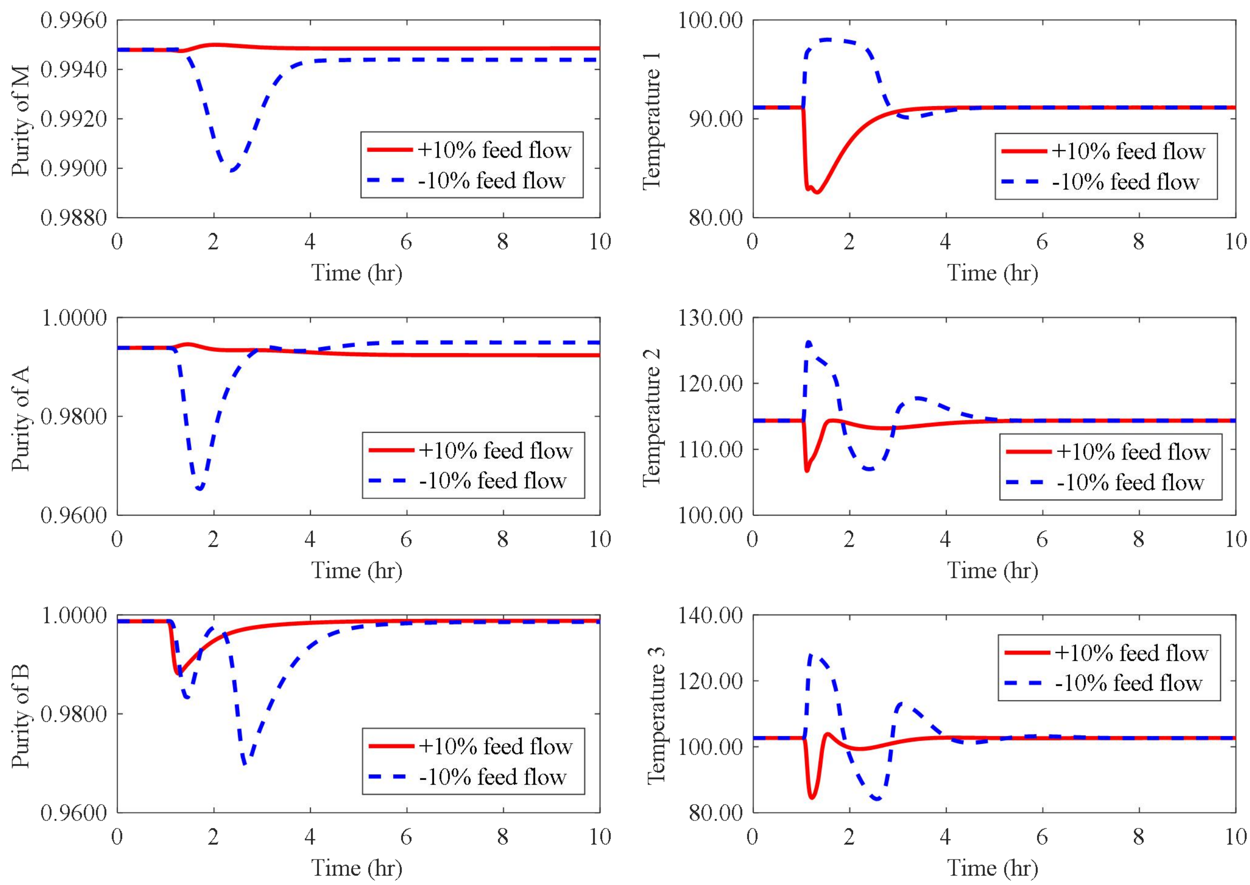

Fig. 4. Dynamics performances of CS1 under ±10% feed flow rate disturbances

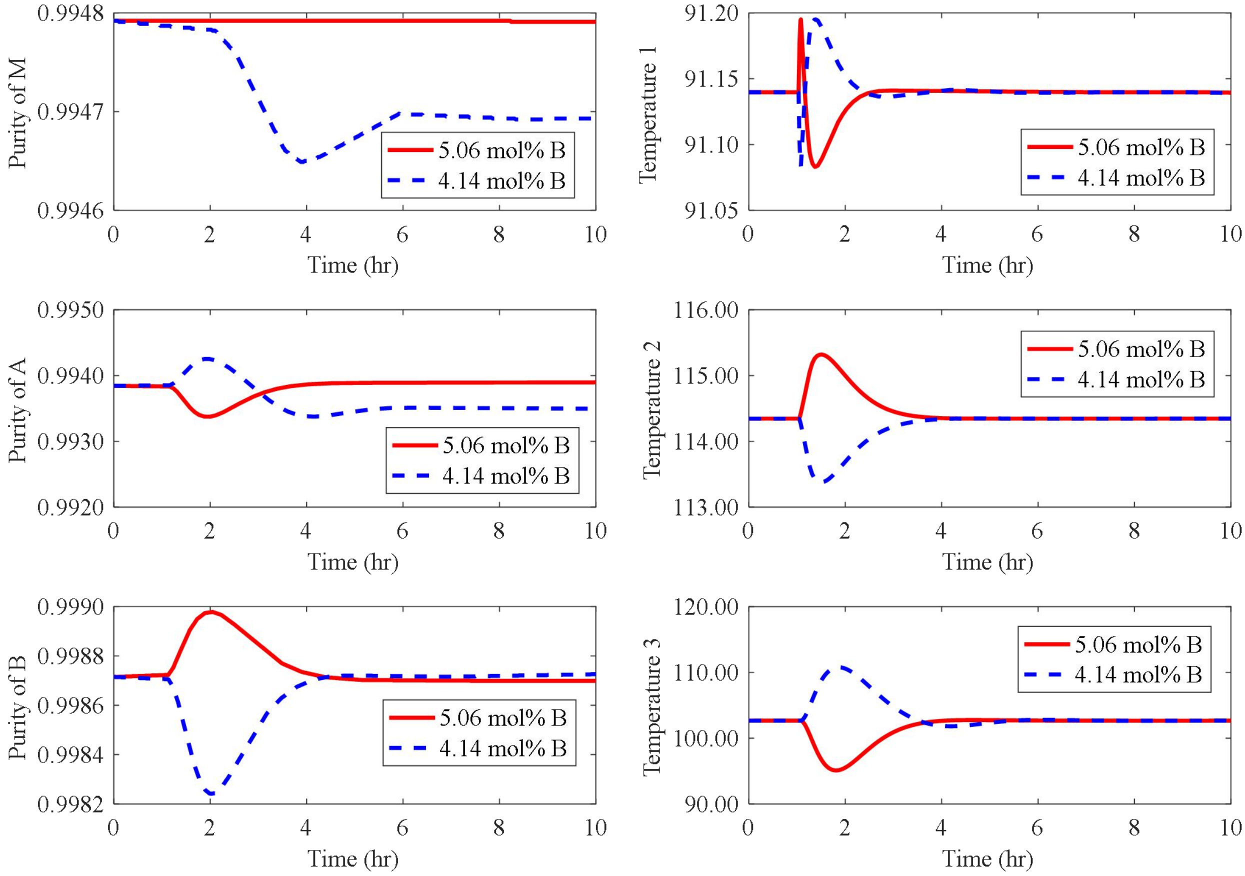

Fig. 5. Dynamics performances of CS1 under ±10% feed composition disturbances

Dynamic responses of the basic control scheme CS1 are evaluated when the ±10% feed flowrates and compositions disturbances are introduced at 1h and terminated at 10h, which is demonstrated in Figures 4 and 5. Of note is that purities of products acetonitrile, methanol and benzene could not back to the specified value at a new stable condition and they have large instantaneous vibration when a -10% feed flow rates disturbance is added. The component methanol is distillated to columns SEDC and SSRC through side-stream. Therefore, it is out of the question for acetonitrile and benzene to be purified in columns SEDC and SSRC. To achieve efficient control, several modified control strategies should be further investigated.

3.3 Control scheme CS2 with feed/side-stream (F/SS) ratio

In view of the weakness of the control structure CS1, it is necessary to explore control scheme of the key factor (i.e., side-stream) to achieve better performance. Control structure CS2 of DSTED with feed/side-stream (F/SS) ratio is proposed based on the CS1. Two F/SS multipliers are added to manipulate the ratio of the side-stream and feed flow rates. Four temperature controllers of the CS2 are retuned and the tuning results are listed in Table 2.

Table 2. Tuning parameters of CS2 for DSTED process

	TC1	TC2	TC3	TC4
Ultimate gain, Ku	1.4551	2.1423	1.2206	0.5288
Ultimate period, Pu (min)	9.6000	13.8000	11.4000	4.2000
Gain, K_C	0.4547	0.6695	0.3814	0.1621
Integral time, τ_I (min)	21.1200	30.3600	25.0800	9.2400

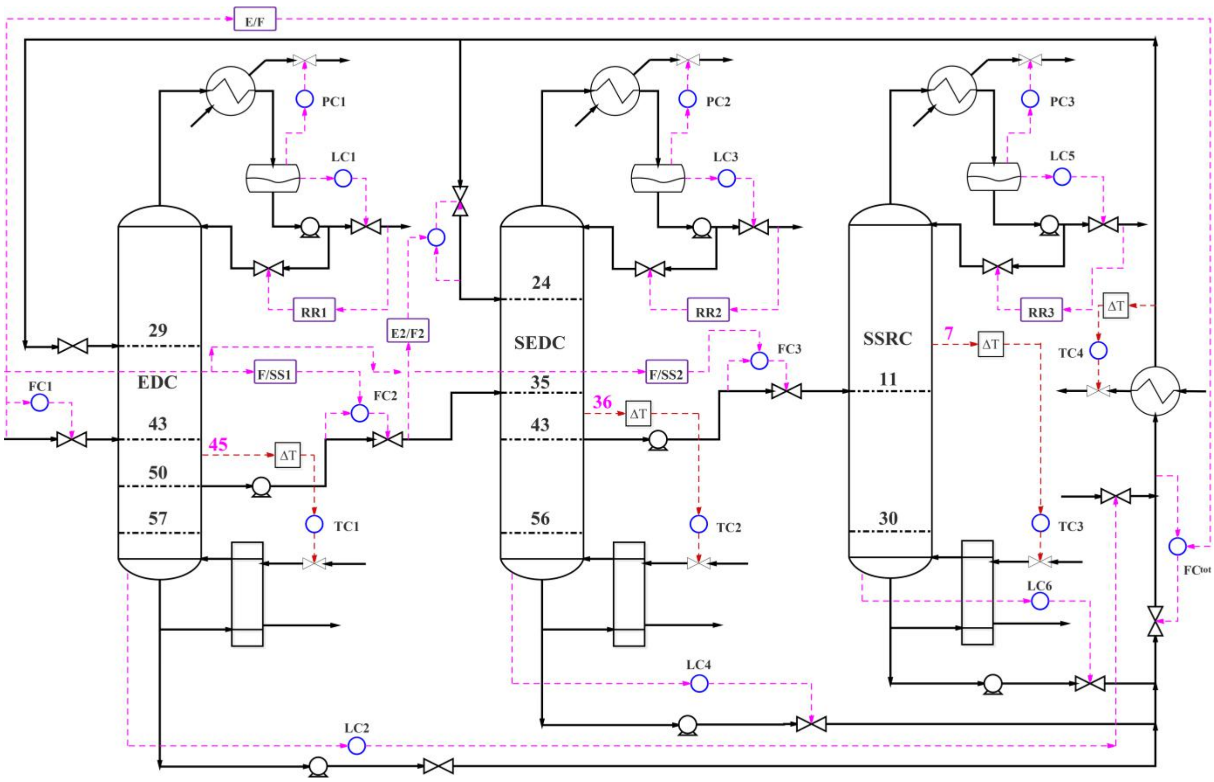

Fig. 6. Control structure CS2 of DSTED with F/SS ratio

Fig. 6 gives the control structure CS2 of DSTED with F/SS ratio. Two multipliers (F/SS1 and F/SS2) are added in the control scheme CS2. Two side-stream flow controllers (FC2 and FC3) are in cascade. ±10% feed flow rates and compositions disturbances are introduced at t = 1 h to assess the performance of control strategy with F/SS.

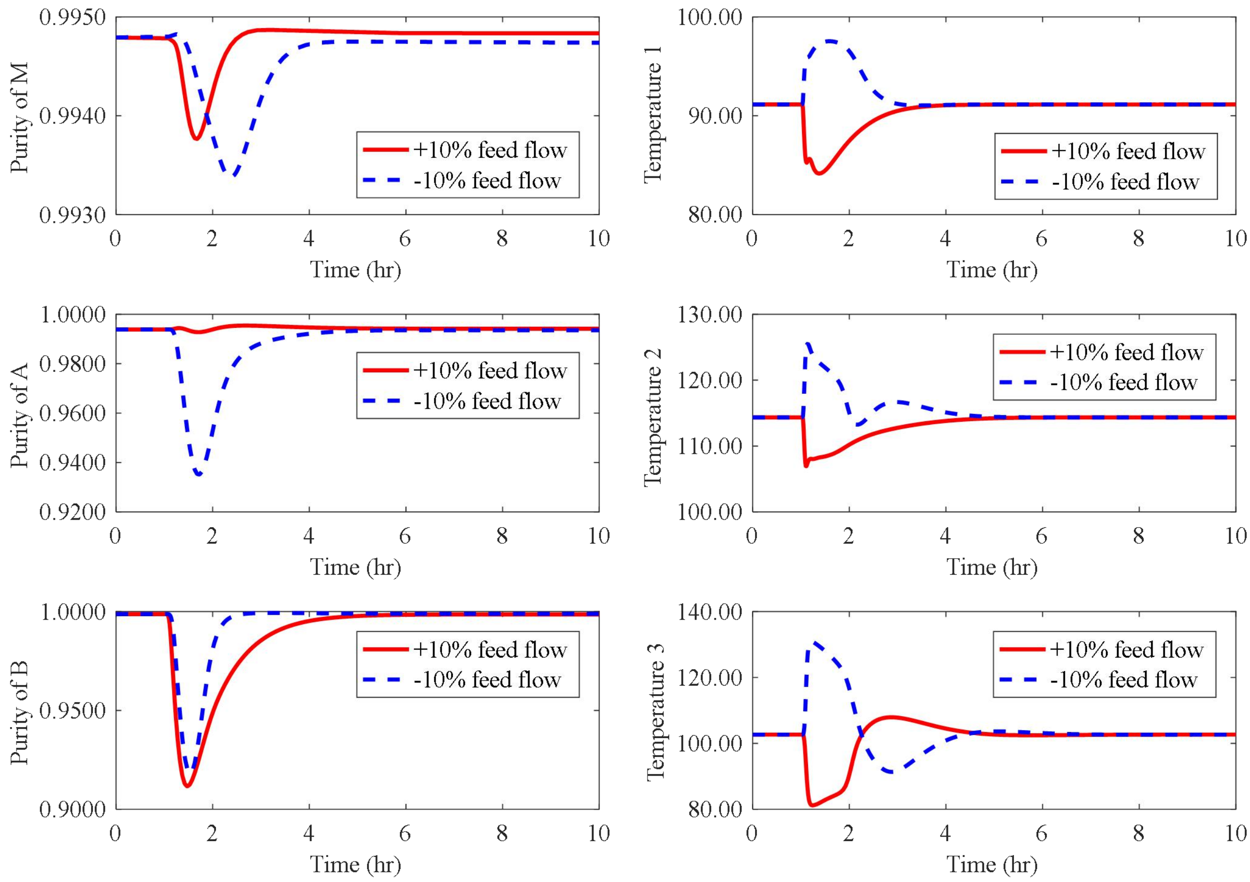

Fig. 7. Dynamics performances of CS2 under ±10% feed flow rate disturbances

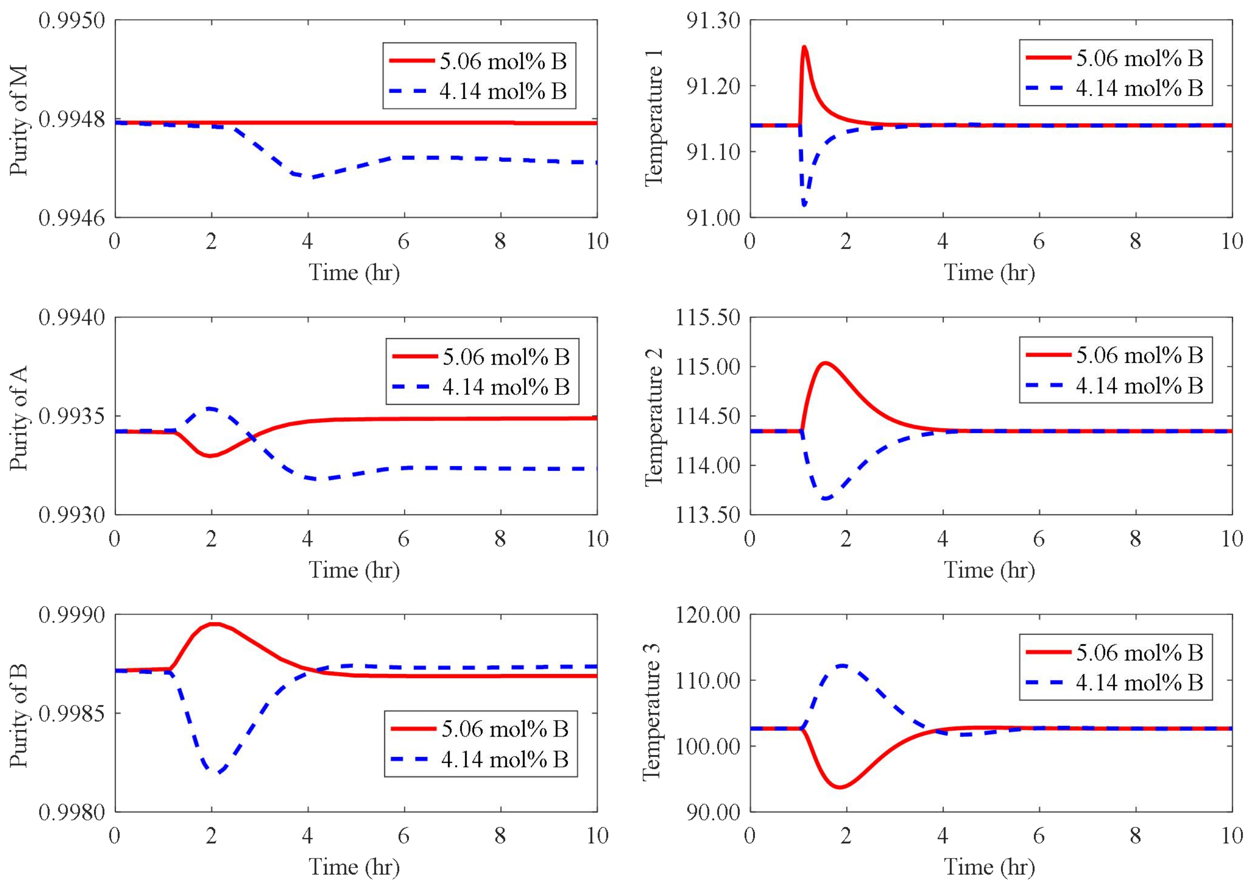

Fig. 8. Dynamics performances of CS2 under ±10% feed composition disturbances

The dynamic response results are demonstrated in Fig. 7 and Fig. 8. Product purities of three columns have large instantaneous vibration at a new state when ±10% flow rates disturbances are added. Compared to the dynamic performance of basic control structure CS1, the CS2 structure with a fixed F/SS ratio received unfavorable control outputs. Therefore, two feedforward control structures are required to be further studied based on the control strategies CS1 and CS2.

3.4 Feedforward control strategy CS3 with F/SS ratio

Following the suggestion of Luyben [3], the feedforward control strategy can effectively reduce the instantaneous vibration to achieve better dynamic controllability for this similar energy-saving process. Therefore, feedforward control structure CS3 of DSTED with F/SS ratio is studied and shown in Fig. 9.

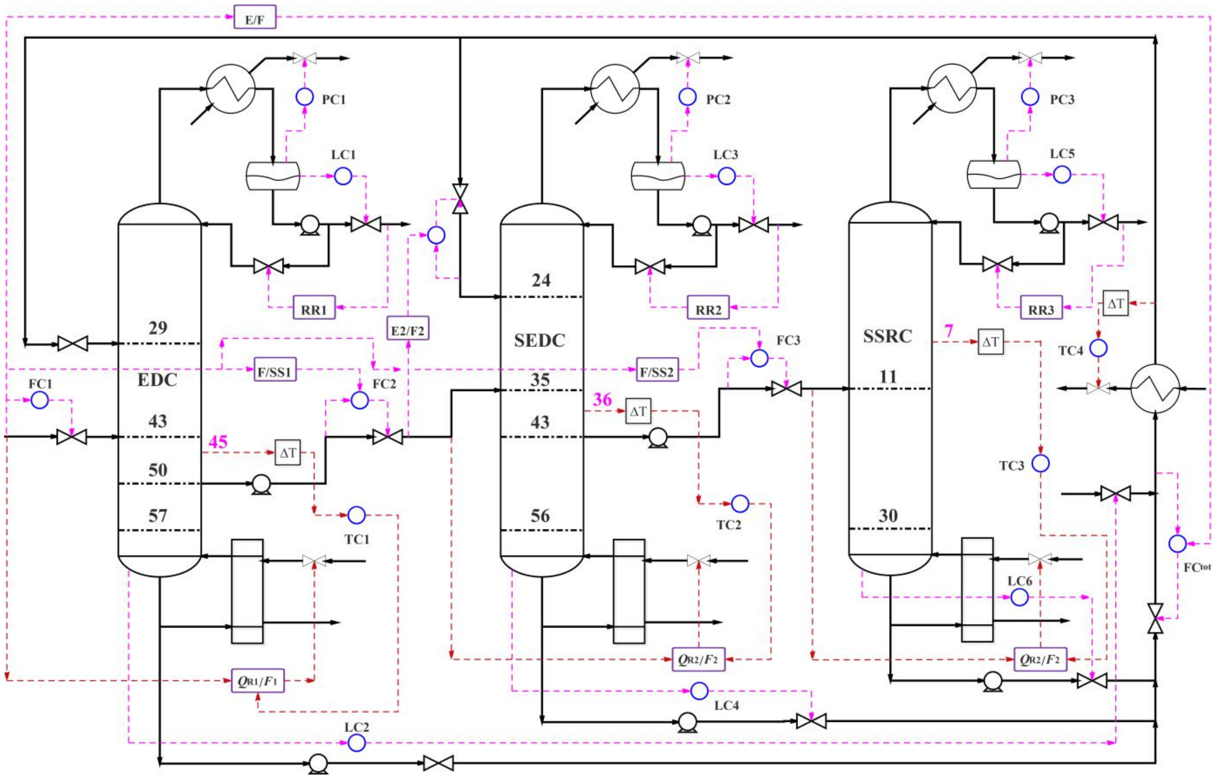

Fig. 9. Feedforward control structure CS3 of DSTED with F/SS

Temperatures of three sensitive trays are controlled via three temperature controllers (TC1, TC2 and TC3) to manipulate the ratios of flowrates and reboiler duties (i.e., Q_{R1}/F_1, Q_{R2}/F_2 and

Q_{R3}/F_3) in the control strategy CS3. Table 3 gives the parameters of temperature controllers in control strategy CS3.

Table 3. Tuning parameters of CS3 for DSTED process

	TC1	TC2	TC3	TC4
Ultimate gain, Ku	1.3732	2.2134	1.5810	0.5185
Ultimate period, Pu (min)	10.2000	14.4000	9.6000	3.6000
Gain, K_C	0.4291	0.6917	0.4941	0.1620
Integral time, τ_I (min)	22.440	31.6800	21.1200	9.2400

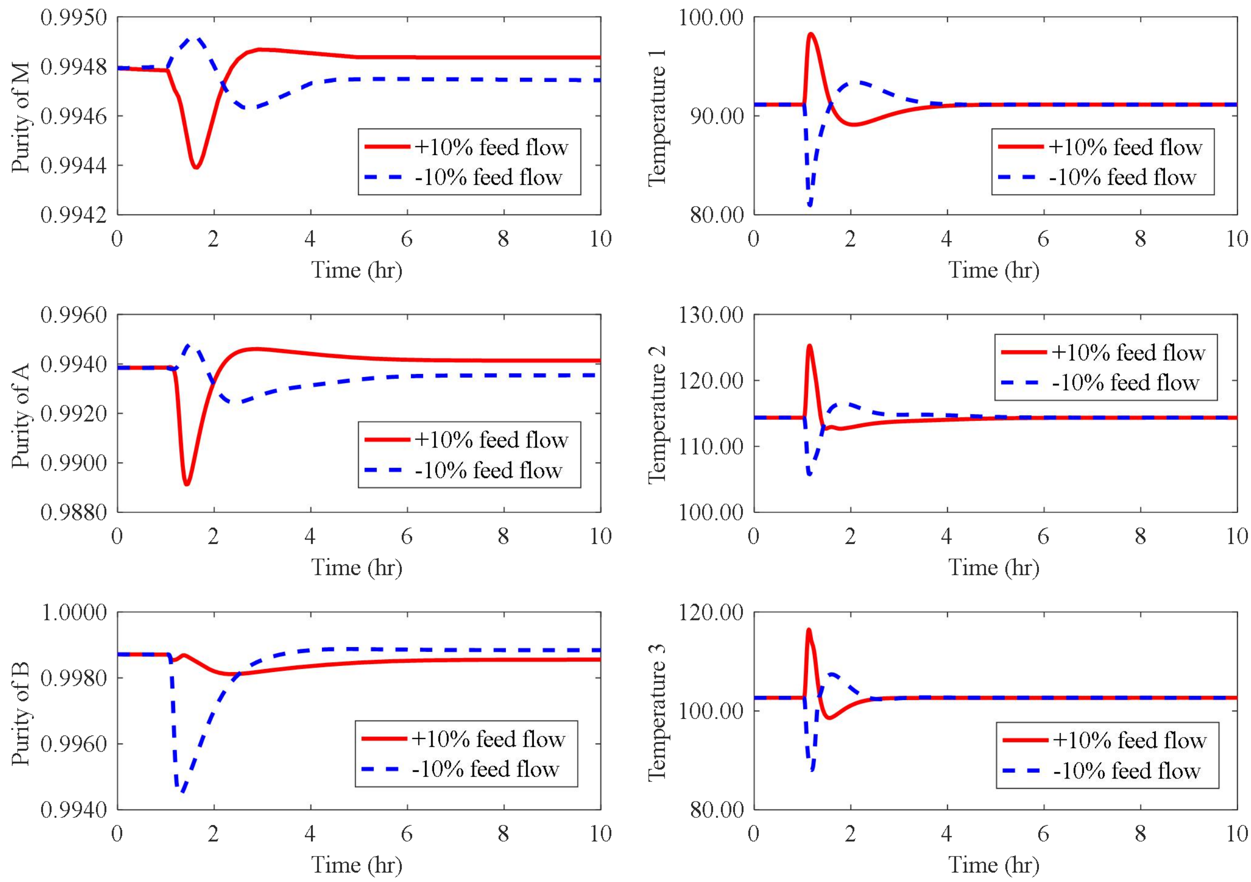

Fig. 10. Dynamics performances of CS3 under ±10% feed flow rate disturbances

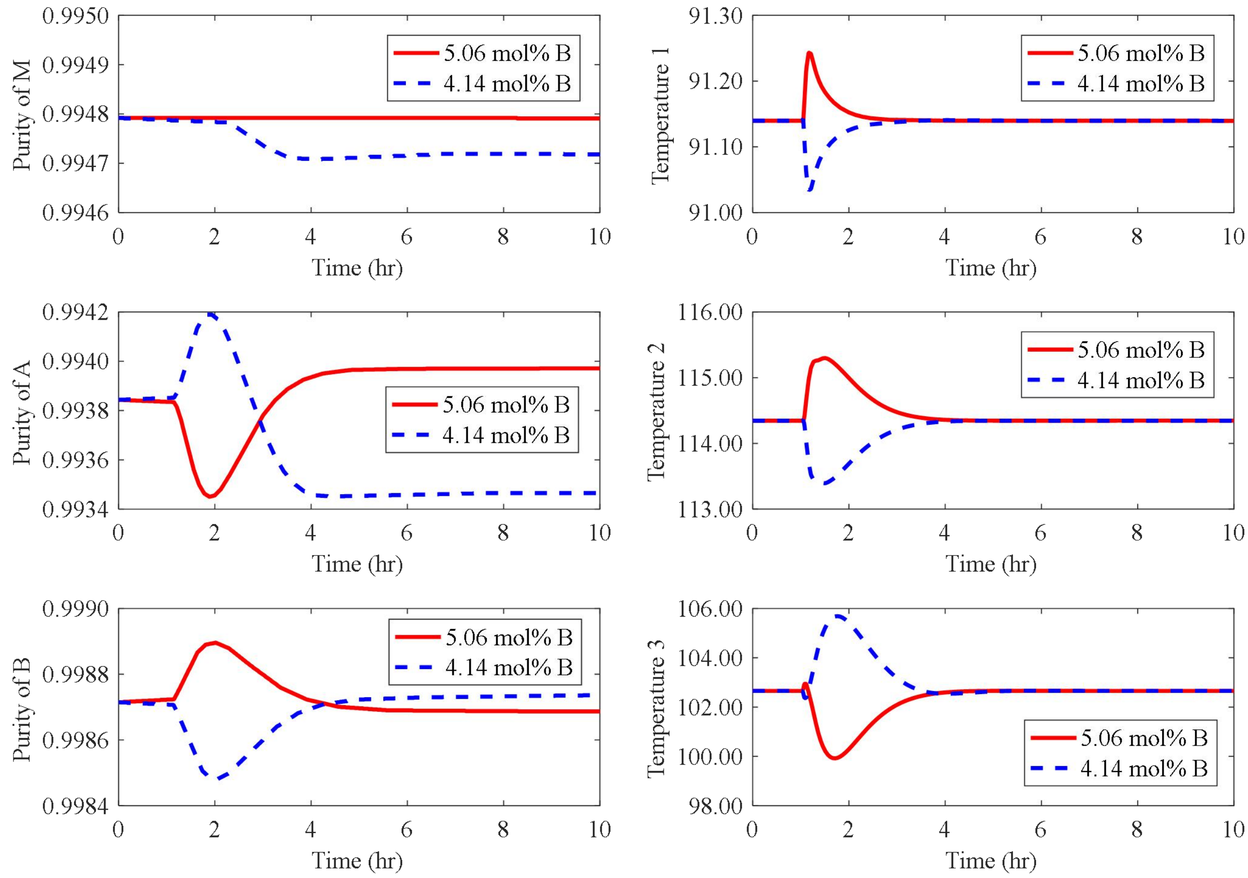

Fig. 11. Dynamics performances of CS3 under ±10% feed composition disturbances

Dynamics performances of control structure CS3 for the DSTED process are exhibited in Figs. 10 and 11. Compared to the dynamic responses of CS1 and CS2, the control performances of CS3 with F/SS ratio have a significant improvement while inevitable disturbances (i.e., ±10% feed flow rates and composition) are introduced. However, the instantaneous vibrations of product purities acetonitrile and benzene under -10% and +10% feed flow rates disturbances are not the desired values. Hence, an improved robust control strategy is further investigated to better handle the product purities.

3.5 Improved feedforward control structure CS4 without F/SS ratio

An improved feedforward control strategy CS4 without F/SS ratio is explored to effectively handle the fluctuation of products purities. Control scheme CS4 of the DSTED sequence is demonstrated in Fig. 12. Integral time and gains of temperature controllers are retuned and the results are demonstrated in Table 4.

Table 4. Tuning parameters of CS4 for DSTED process

	TC1	TC2	TC3	TC4
Ultimate gain, Ku	1.4037	2.0339	1.0521	0.5164
Ultimate period, Pu (min)	10.2000	14.4000	12.0000	3.6000
Gain, K_C	0.4387	0.6356	0.3288	0.1614
Integral time, τ_I (min)	22.4400	31.6800	26.4000	7.9200

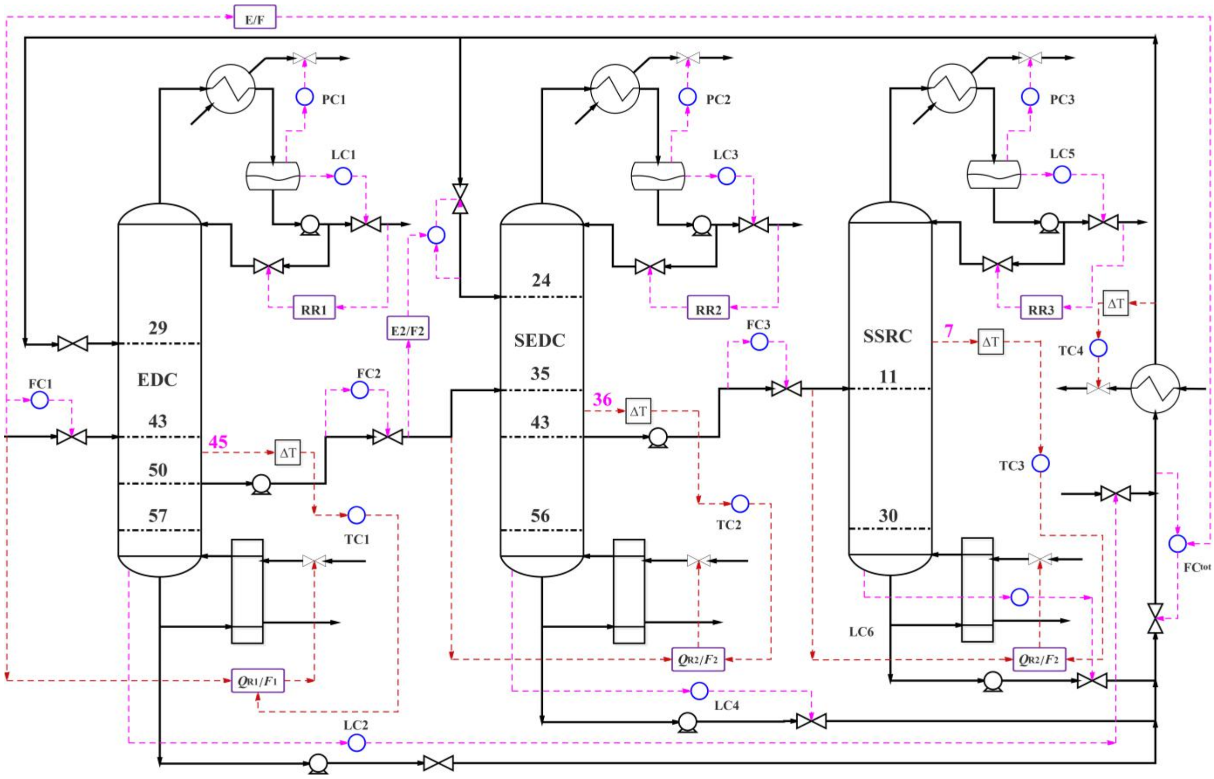

Fig. 12. Improved feedforward control structure CS4 of DSTED without F/SS

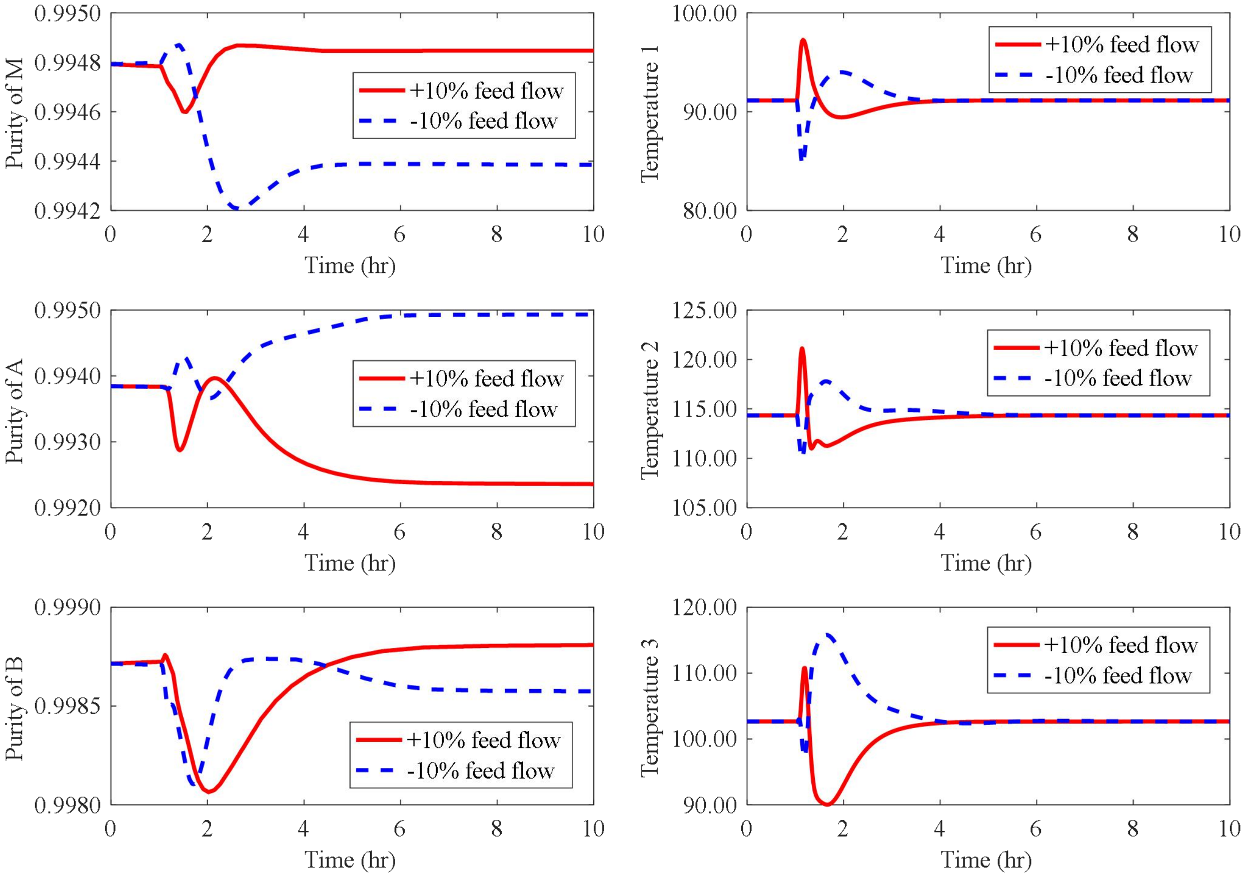

Fig. 13. Dynamics performances of CS4 under ±10% feed flow rate disturbances in fresh feed

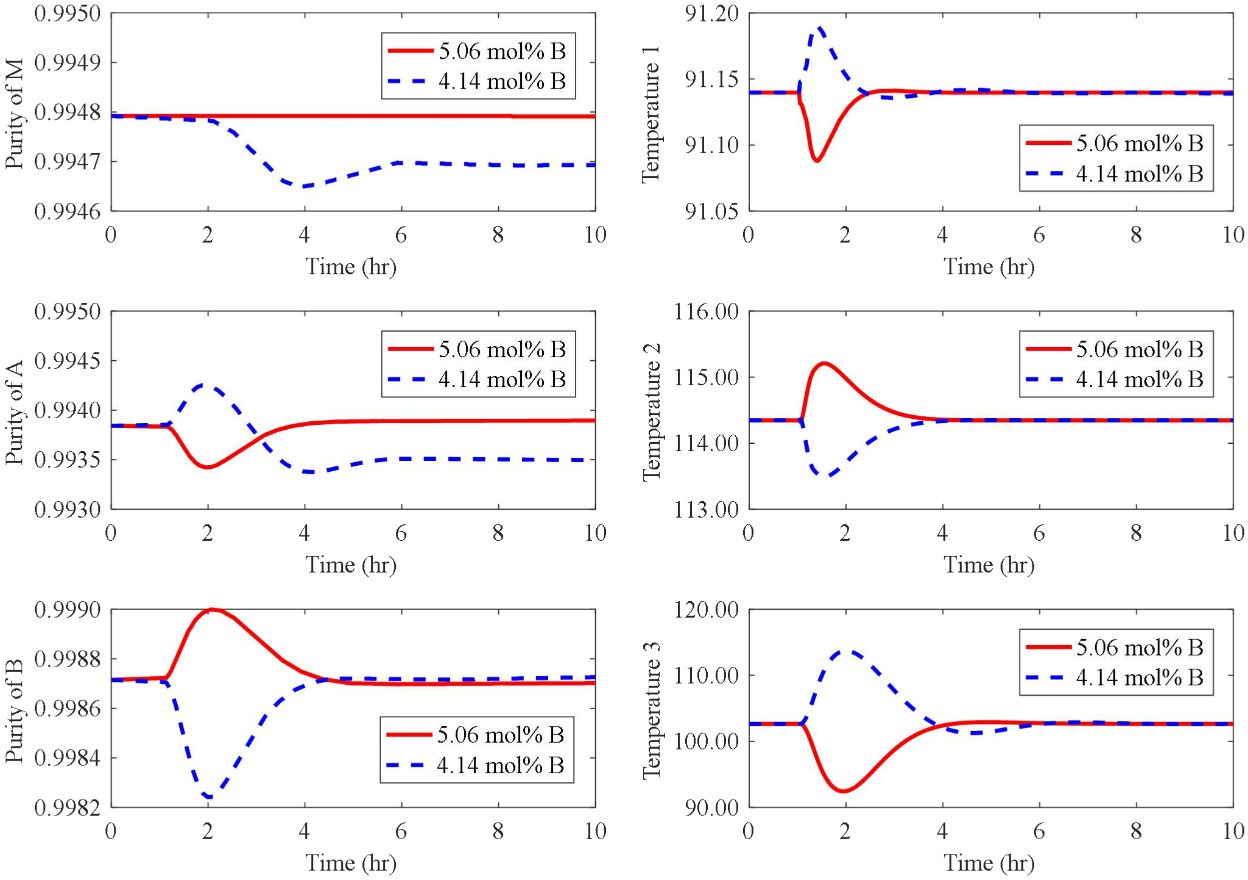

Fig. 14. Dynamics performances of CS4 under ±10% feed composition disturbances in fresh feed

Figs. 13 and 14 illustrate the dynamic characteristic of the robust control strategy CS4 under ±10% feed flow rates and compositions disturbances. The product purities could be quickly gotten back to their desired values (i.e., 5h) under fresh feed flow rates disturbances. In addition, desired products purities of acetonitrile, benzene and methanol could also be obtained about 4h under feed composition disturbance. Meanwhile, the instantaneous vibrations of product purities are reduced to achieve the desired values. In summary, responses of the robust control scheme CS4 are the best than the previous three control strategies CS1, CS2 and CS3 for the intensified DSTED scheme.

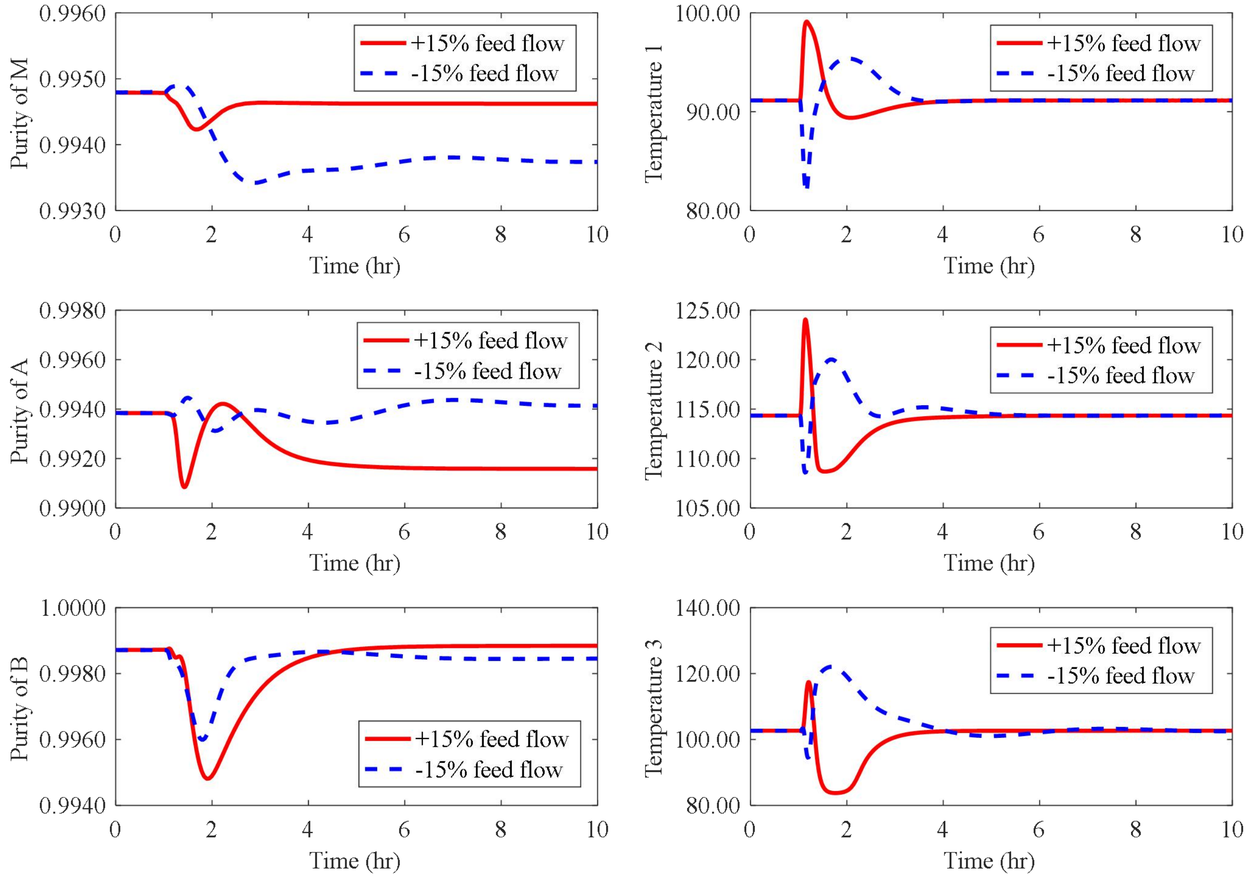

Fig. 15. Dynamics performances of CS4 under ±15% feed flow rate disturbances in fresh feed

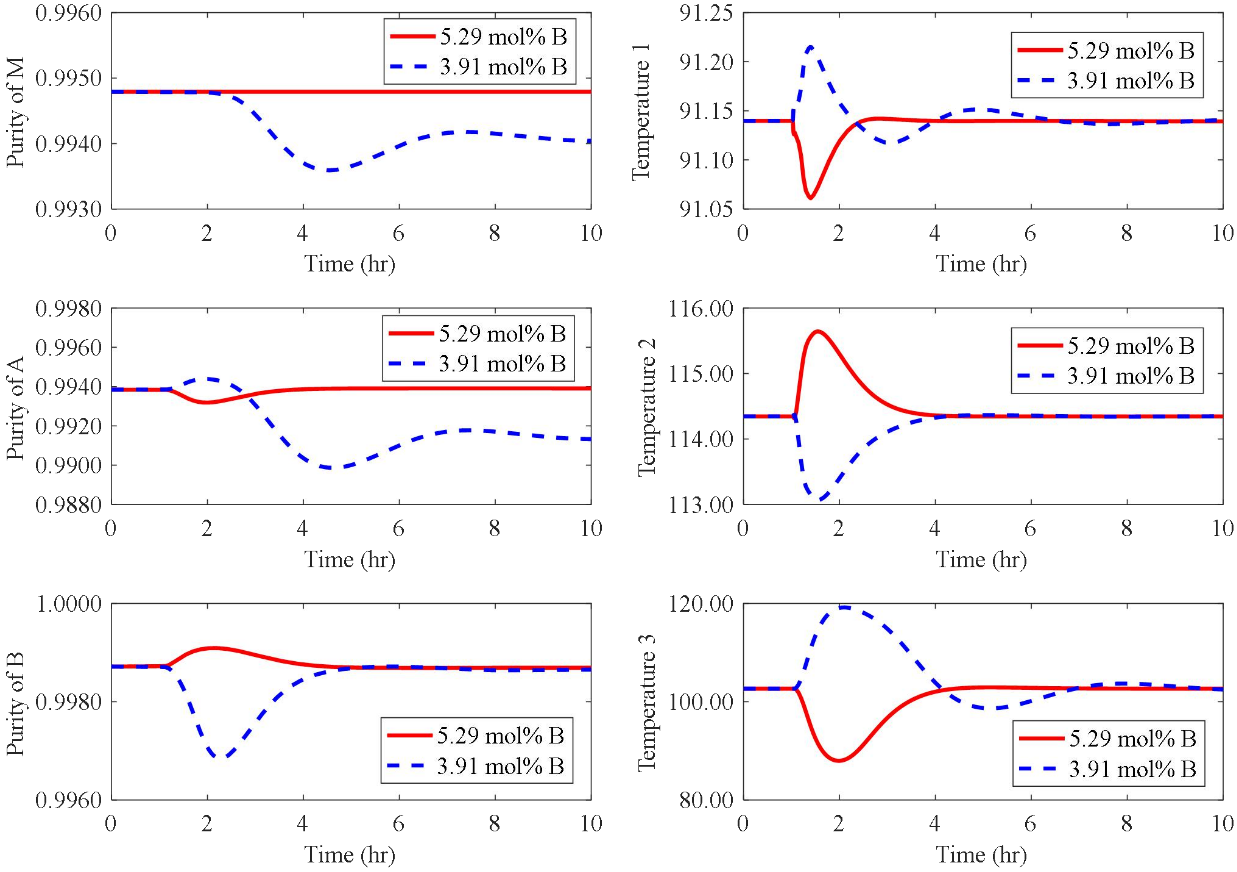

Fig. 16. Dynamics performances of CS4 under ±15% feed composition disturbances in fresh feed

Moreover, additional ±15% feed flow rates and compositions disturbances are added in the control strategy CS4 to evaluate the stability and controllability of the DSTED. Fig. 15 and Fig. 16 give the dynamic performance of the improved control strategy CS4 handling ±15% disturbances. In a word, larger disturbances for ternary mixtures could also be well handled in real chemical processes.

4. Discussion and Comparison

To design a robust control strategy, more attention should be focused on the side-stream in DSTED scheme. Therefore, two control structures CS1 and CS2 with or without F/SS ratio are explored and compared. Dynamic performances illustrate that CS1 and CS2 cannot effectively control the product purities when ±10% feed disturbances are added in the fresh feed. However, purities of three columns have large instantaneous vibration. Hence, two feedforward control structures CS3 and CS4 are presented to improve the control performances. Dynamic responses of two improved control schemes illustrate that the improved robust control structure CS4 without F/SS ratio can effectively handle the product purities by adding flow rates and compositions disturbances. The dynamic response for confronted feed flow rates and composition disturbance reach stable-state after 5h and 4h, respectively. In addition, ±15% feed disturbances are implemented to further vitrify the dependability of the developed control scheme (see Figs. 15 and 16). Control structure CS4 exhibits exact controllability dealing with ±15% feed disturbances.

Of note is that, a composition control structure with a long delay time and expensive gas chromatographic equipment is studied to achieve a new steady-state with a long vibration time (about 15 and 5h for flow rate and composition disturbances). In this work, a robust temperature control scheme with cheap temperature measuring equipment (i.e., fast response) is proposed to maintain three product purities with a short vibration time (about 3 and 7h for two kinds of disturbances).

5. Conclusion

In this work, four control schemes are explored to achieve robust control of the energy-saving double side-streams ternary extractive distillation (denoted as DSTED). The basic control structures with or without F/SS ratio (CS1 and CS2) cannot achieve control performances effectively because of the complexity of the energy-saving DSTED process. Hence, two improved control strategies (CS3 and CS4) with Q_R/F ratio are then studied. It is observed that product purities of feedforward control structure CS4 could be well controlled confronting ±10% feed flow rates and compositions disturbances. Furthermore, additional ±15% feed disturbances are added in the CS4 to assess the stability and controllability of the DSTED scheme. Larger disturbances for ternary mixtures could also be handled in real chemical processes. In summary, this study will push forward the application of energy-saving DSTED.

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Notes

The authors declare no competing financial interest.

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