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Research Article

Separating Mixture Glycols in DWC with Flow Rate-Composition Cascade Control Structure

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Dividing wall column (DWC) is an advanced technology which could decrease energy consumption. As the vertical wall inserted in DWC increases the degree of freedom of systems, the control becomes more difficult than the conventional columns. In this study, the mixture glycols (1, 2-propanediol+ 1, 3-butanediol+ 1, 4-butanediol) were taken as feed, an optimized DWC structure was proposed, and three control structures for DWC were tested by ± 10% feed disturbances. The temperature control structure (CS1) was hard to control the system while composition control structure (CS2) and flow rate-composition cascade control structure (CS3) had good performance on controlling the DWC. It showed that CS3 was superior to CS2, as CS3 could stabilize the DWC within 4 hours, and the maximum deviations of the three products, namely 1, 2-propanediol, 1, 3-butanediol and 1, 4-butanediol, were 0.07%, 1.44%, and 0.46% respectively, while CS2 could realize the stability within 7 hours, and the corresponding numbers were 0.35%, 2.78%, and 0.41%, respectively.

1. Introduction

Distillation is the most widely used technology to separate mixtures in chemical industry, and about 95% of liquid mixtures are separated by distillation [1, 2]. However, it is an energy-intensive process, which accounts for an estimated 3% of the energy consumption in the world [2–4]. In order to decrease the energy requirements in distillation, several technologies have been proposed, such as heat pump assisted distillation column, internally heat integrated distillation column, and fully thermally coupled column (Petlyuk column).

DWC is thermodynamically equivalent to and further a practical implementation of the Petlyuk column. A vertical wall which splits the column into two sections is inserted in DWC. The feed enters into the prefractionator side, and the side product leaves column from the opposite side of the wall, which is called as the main fractionator. The component with low boiling point is removed from the top while the one with high boling point is removed from the bottom. DWC only needs a single tower with one reboiler and one condenser for separation of multicomponent mixtures. In the meanwhile, the thermal efficiency improves because the remixing effect could be highly decreased by the vertical wall [5]. It is reported that DWC could reduce almost 30% of energy consumption and also 30% capital costs in comparison to an ordinary distillation sequence [5–9]. DWC was first applied in industry by BASF in 1985 [10]. In 2010, there were over 100 DWCs reported in operation [7, 11], most of which were run by BASF. However, DWCs still accounted for a minor proportion compared to the over 40,000 conventional distillation columns in chemical industry [12].

It is generally considered that intensified processes, like DWC, are more difficult to be controlled than conventional processes due to the following: (a) the more degree of freedom than a conventional distillation column, (b) the highly nonlinear behavior caused by the complicated structure, and (c) the strong interactions between manipulated and controlled variables [5, 13–17]. Dynamic control is one of the keys to the operation of DWC.

Several control structures have been tested in the open literature, such as temperature control structure, composition control structure, temperature difference control (TDC) structure, temperature-composition cascade control structure, model predictive control (MPC) structure, and so on. Some have been applied into the separation of the systems, like alcohols, alkanes, and aromatics. The control structures usually take reflux ratio (RR), reboiler duty (Q_R), and side product flow rates (S) as manipulated variables. Liquid split ratio is an optional manipulated variable for the control of the heavy component at the top of the prefractionator [18, 19].

Composition control structure takes composition, reflux drum level, and sump level of column as controlled variables. It can deal with feed disturbances and return to steady state in 2~10 hr [12, 18–36], while sometimes it takes a long time to get steady [24, 33, 35].

Different from composition control structure, temperature control structure takes the temperatures at reference stages as manipulated variables. It can deal with feed disturbances and return to steady state in 2~5 hr [37–48]. Temperature control structure responds fast to disturbances, but sometimes the purity of products may have big deviations [43, 45, 49].

Composition-temperature cascade control structure can overcome long time delays caused by composition controllers and deal with feed disturbances with small deviations. The system with the structure can recover to steady state in 2~6 hr [49, 50]. The cascade control structure still has a high cost and it is difficult to be tuned because of its complexity.

TDC structure adds additional temperature measurements into temperature control structure in order to get a better performance on dealing with feed disturbance, especially for the feed composition disturbance. TDC structure can deal with feed disturbances in 2~5 hr [16, 51–56]. Although TDC always has better performance than temperature control structure, deviations for product purity still exist.

MPC structure is an advanced control structure, and it is an optimization based on multivariable constrained control technology [57]. Adrian et al. [58] compared MPC with conventional PI control in DWC. MPC structure shows a tighter and faster control than PI control. It can deal with feed disturbances in 2~8 hr [17, 26, 57–62]. However, MPC is hard to implement and needs more efforts than PI control [15, 57].

Glycols including 1, 2-propanediol, 1, 3-butanediol, and 1, 4-butanediol with a wide application could be used as biofuels which are considered promising alternative energy [63, 64]. They have some unusual properties, such as availability, nonvolatility, nontoxicity, and biodegradability. Such advantages make a promising application of 1, 2-propanediol, 1, 3-butanediol, and 1, 4-butanediol into the production of polyester fibers, antifreeze materials, packaging materials, engineering plastics, and surfactants [65–67]. However, the separation becomes one of the keys to the industrial applications of the bio-glycols.

Several groups of vapor-liquid equilibria data of glycols were studied in the literature [68–70]. In this paper, the separation of mixture glycols (1, 2-propanediol+ 1, 3-butanediol+ 1, 4-butanediol) by DWC and three control structures have been studied by ±10% feed disturbances. All of the three structures were based on simple single-loop PI control. This study could provide a potential solution to the systems with similar molecular structures and properties by DWC.

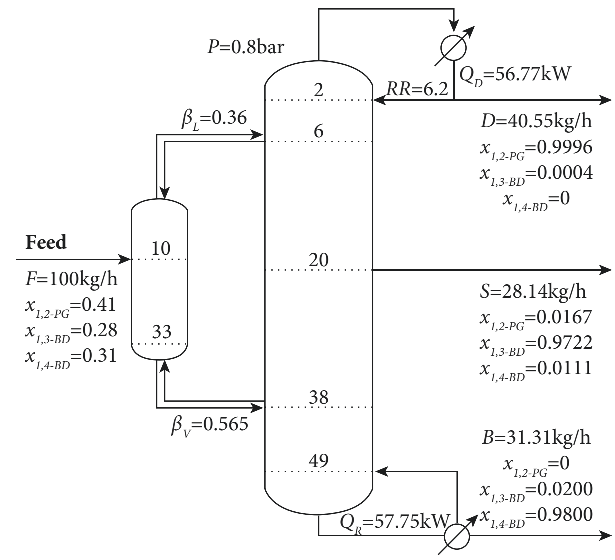

Figure 1: Two-shell configuration of the DWC.

Table 1: Detailed design data of DWC.

	Prefractionator	Main column
Number of stages	33	50
Feed stage	15	6/38
Side product stage	—	20
Mole reflux ratio	—	6.2
Vapor split ratio (β_V)	—	0.565
Liquid split ratio (β_L)	—	0.360
Reboiler duty (kW)	—	57.75
Purity of products (mass%)	—	99.9/97.2/98.0
Mass flow of products (kg/h)	—	40.55/28.14/ 31.31

2. Steady-State Design

The ternary system of 1, 2-propanediol (1, 2-PG) + 1, 3-butanediol (1, 3-BD) + 1, 4-butanediol (1, 4-BD) was studied. The boiling points of the glycols are 460.45 K, 481.38 K, and 501.15 K, and the relative volatilities are 3.74, 2.19, and 1, respectively. A mixture of 41.0 wt% 1, 2-PG, 28.0 wt% 1, 3-BD, and 31.0 wt% 1, 4-BD was taken as feed and its flow rate was set as 100 kg/hr at boiling point. The target purity of 1, 2-PG, 1, 3-BD, and 1, 4-BD was 99.8 wt%, 97.2 wt%, and 98.0 wt%, respectively. Rigorous simulations were carried out by RADFRAC modules in Aspen Plus with the UNIQ-HOC thermodynamic model.

As shown in Figure 1, the simulation used two-shell configuration including a prefractionator and a main column, which was thermodynamically equivalent to the DWC. The number of trays including a condenser and a reboiler was 50 for the main column in DWC. The vertical wall was placed from stage 6 to stage 38 in column. In

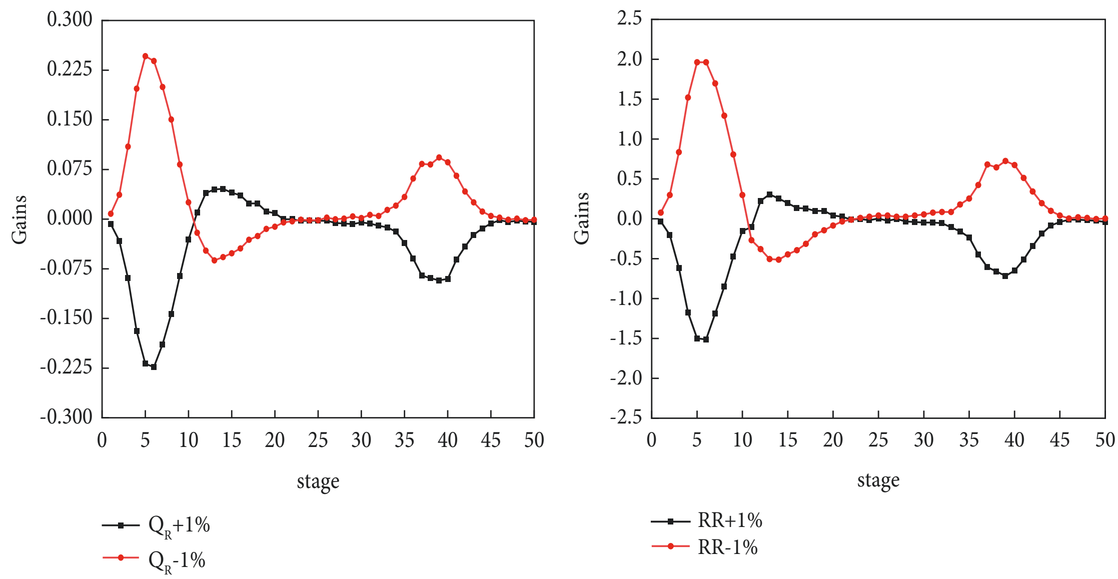

Figure 2: Sensitivity analysis of the main column.

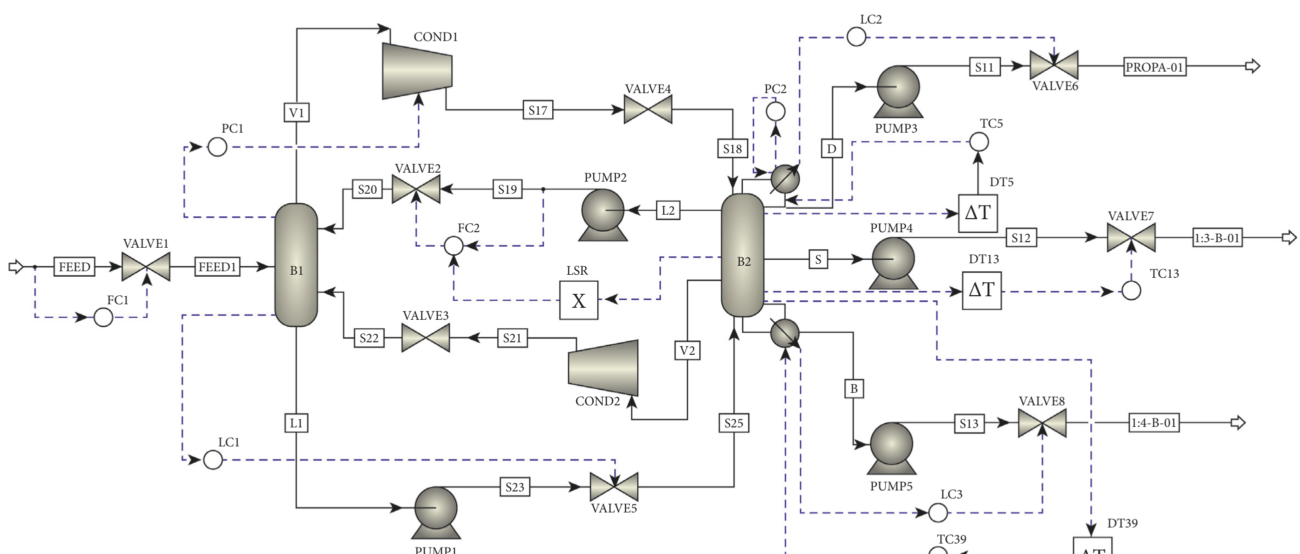

Figure 3: Temperature control structure CS1 of DWC.

order to obtain high-purity products, the pressure of the condenser was set as 0.8 bar and tray pressure drop of 0.0068 atm was considered. Detailed design data for DWC are listed in Table 1.

3. Control Structure Design

3.1. Temperature Control Structure (CS1). Temperature control structure is widely used in industry because it is simple and cheap. In this study, the temperature control structure was first tested for the DWC. Reflux rate (RR), side stream flow rate (S), and reboiler duty (Q_R) were taken as manipulated variables and temperature at reference stages was taken as control variable. In order to find the appreciate reference stages, a small change (+1%) was implemented in an independent variable (RR or Q_R) while keeping the other variables constant. Figure 2 shows the sensitivity analysis for the DWC. Apparently, stages 13 and 39 could be selected as the reference stages for the side stream and stripping sections, respectively. The rectifying section accounted for only 5 theoretical trays, so stage 5 was chosen as reference stage for the rectifying section.

Table 2: Controller tuning parameters of CS1.

Control loop	Controlled variable	Manipulated variable	K_c	τ_I/min
TC5	$T_{mai,5}$	RR	5.244	10.56
TC13	$T_{mai,13}$	S	55.518	29.04
TC39	$T_{mai,39}$	Q_R	2.783	6.60

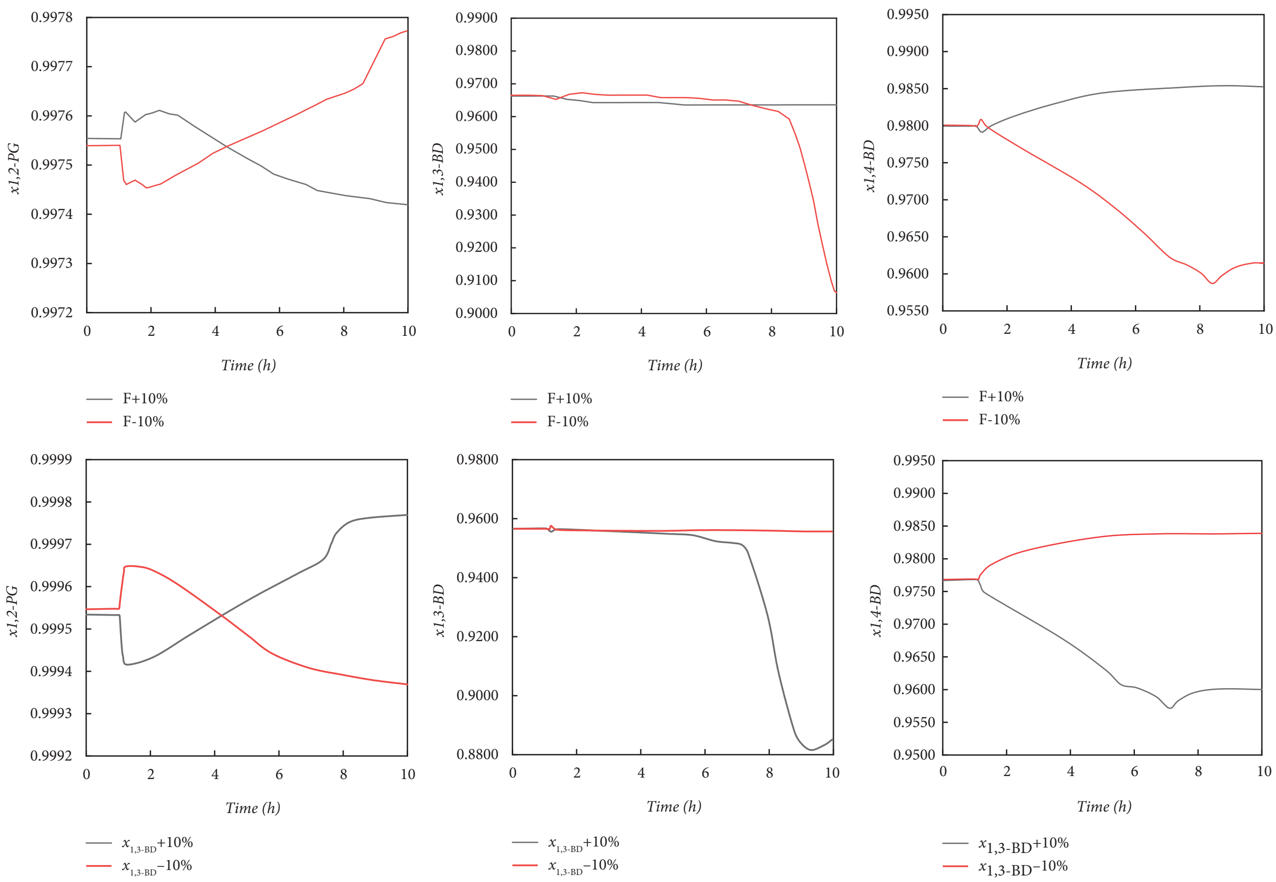

Figure 4: Dynamic responses of CS1 to ±10% feed disturbances.

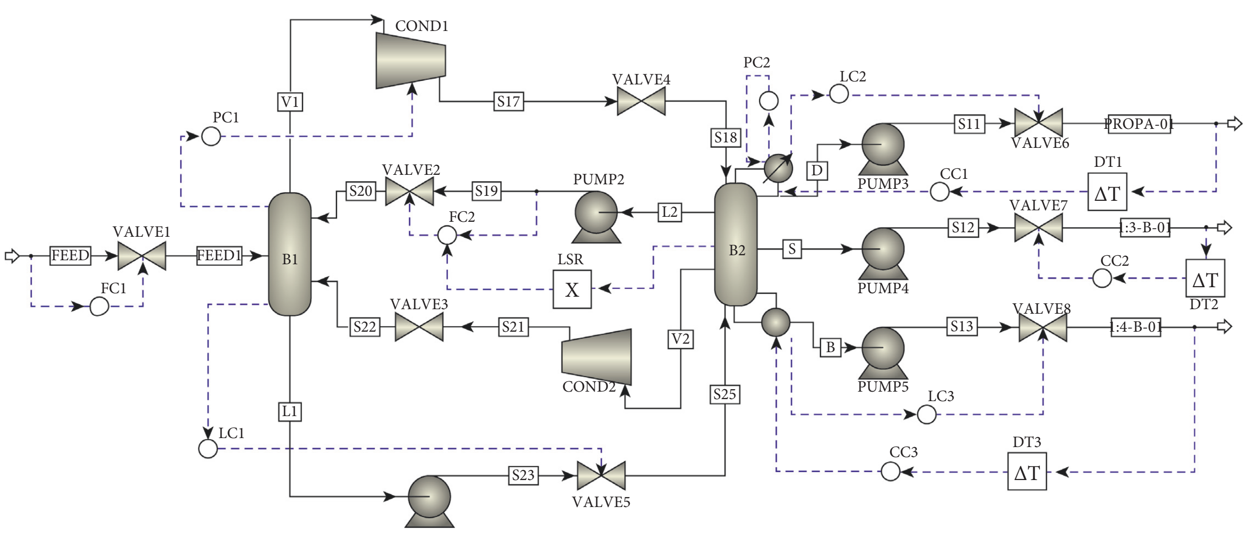

Figure 5: Composition control structure CS2 of DWC.

Figure 3 illustrates CS1 of DWC. The controller labeled TC5 turned the temperature at stage 5 by manipulating RR, the temperature at stage 13 was controlled by S, and Q_R was the manipulated variable for controlling the temperature at reference stage 39 with TC39. The three loops were tuned sequentially, the gain (K_C) and integral time (τ_I) of the temperature controllers were obtained through the relay-feedback test and Tyreus–Luyben tuning method, and the dead time for temperature controllers was set as 1 min. Table 2 gives the detailed temperature controller parameters in CS1. To complete CS1, Kc and τ_I were 0.5 and 0.3 min for the flow controllers, respectively, 20 and 12 min for the

Table 3: Controller tuning parameters of CS2.

Control loop	Controlled variable	Manipulated variable	K_c	τ_I/min
CC1	$x_{1,2-PG}$	RR	1.766	91.08
CC2	$x_{1,3-BD}$	S	10.838	112.20
CC3	$x_{1,4-BD}$	Q_R	2.801	30.36

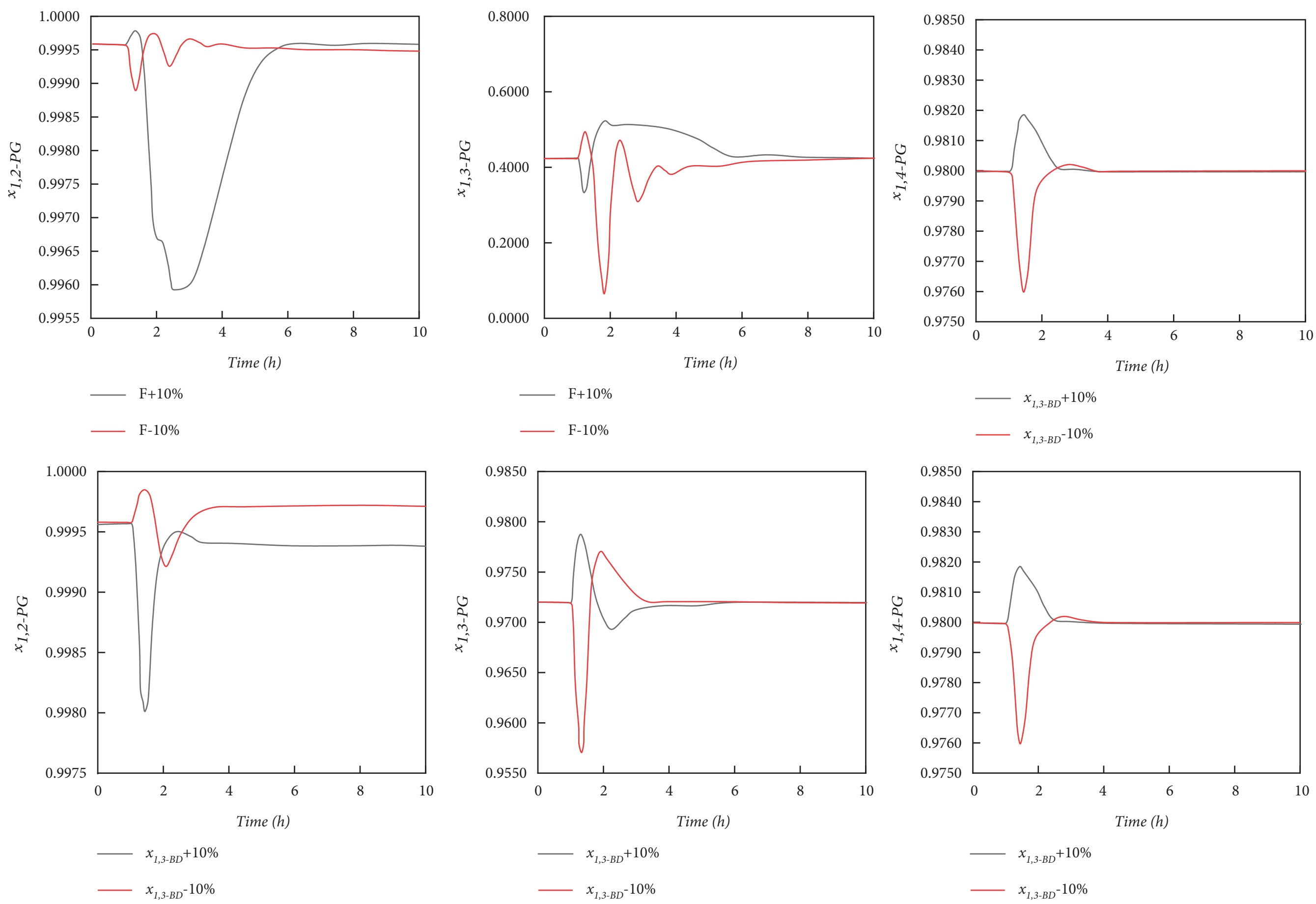

Figure 6: Dynamic responses of CS2 to ±10% feed disturbances.

pressure controllers, respectively, and 2 and 9999 min for liquid level controllers, respectively.

Figure 4 shows the responses of CS1 under ±10% feed disturbances. Apparently, the control structure showed a poor control performance on dealing with the disturbances; the purity of all the three products presented big deviations after 10hr, especially for the side stream 1, 3-BD.

3.2. Composition Control Structure (CS2). CS2 adopted composition controllers instead of temperature controllers. As shown in Figure 5, the controller CC1 maintained the purity of 1, 2-PG by manipulating RR, CC2 maintained the purity of 1, 3-BD by manipulating S, and CC3 maintained the purity of 1, 4-BD by manipulating Q_R. The set dead time for composition controllers was 3 min in consideration of its longer time delay than that in temperature controller. The detailed parameters for composition controllers obtained by the relay-feedback test and Tyreus–Luyben tuning method are listed in Table 3, and the other controllers used the same parameters as CS1.

Figure 6 illustrates the dynamic responses of CS2 under ±10% feed disturbances, and the product purity could get steady within 6 hr with almost same purity to the initial states. The maximum deviations due to feed flow rate disturbances in the purity of 1, 2-PG, 1, 3-BD, 1, 4-BD were 0.35%, 2.78%, and 0.41%, respectively, and the maximum deviations due to feed composition disturbances were 0.15%, 1.54%, and 0.41%, respectively.

3.3. Flow Rate-Composition Cascade Control Structure (CS3). Although CS2 could deal with ±10% feed disturbances well, the long recovery time, maximum deviations, and high expense for composition controllers still needed to be improved. In CS3, a temperature controller was used to

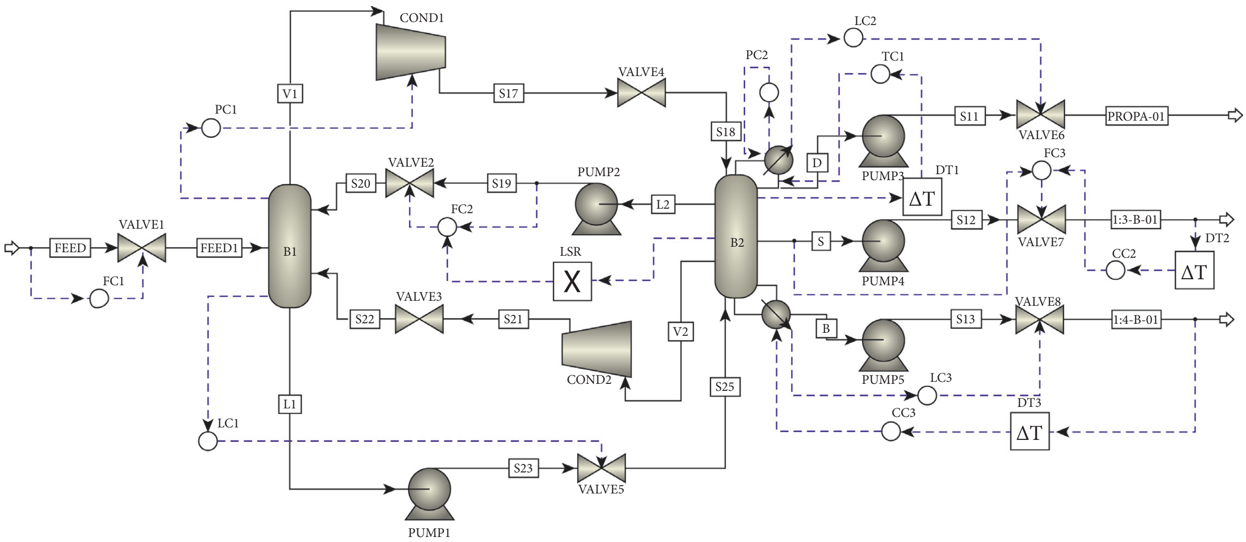

Figure 7: Cascade control structure CS3 of DWC.

Table 4: Controller tuning parameters of CS3.

Control loop	Controlled variable	Manipulated variable	K_c	τ_I/min
TC1	$T_{mai,5}$	RR	6.906	10.56
CC2	$x_{1,3-BD}$	S	18.038	80.52
CC3	$x_{1,4-BD}$	Q_R	2.801	30.36

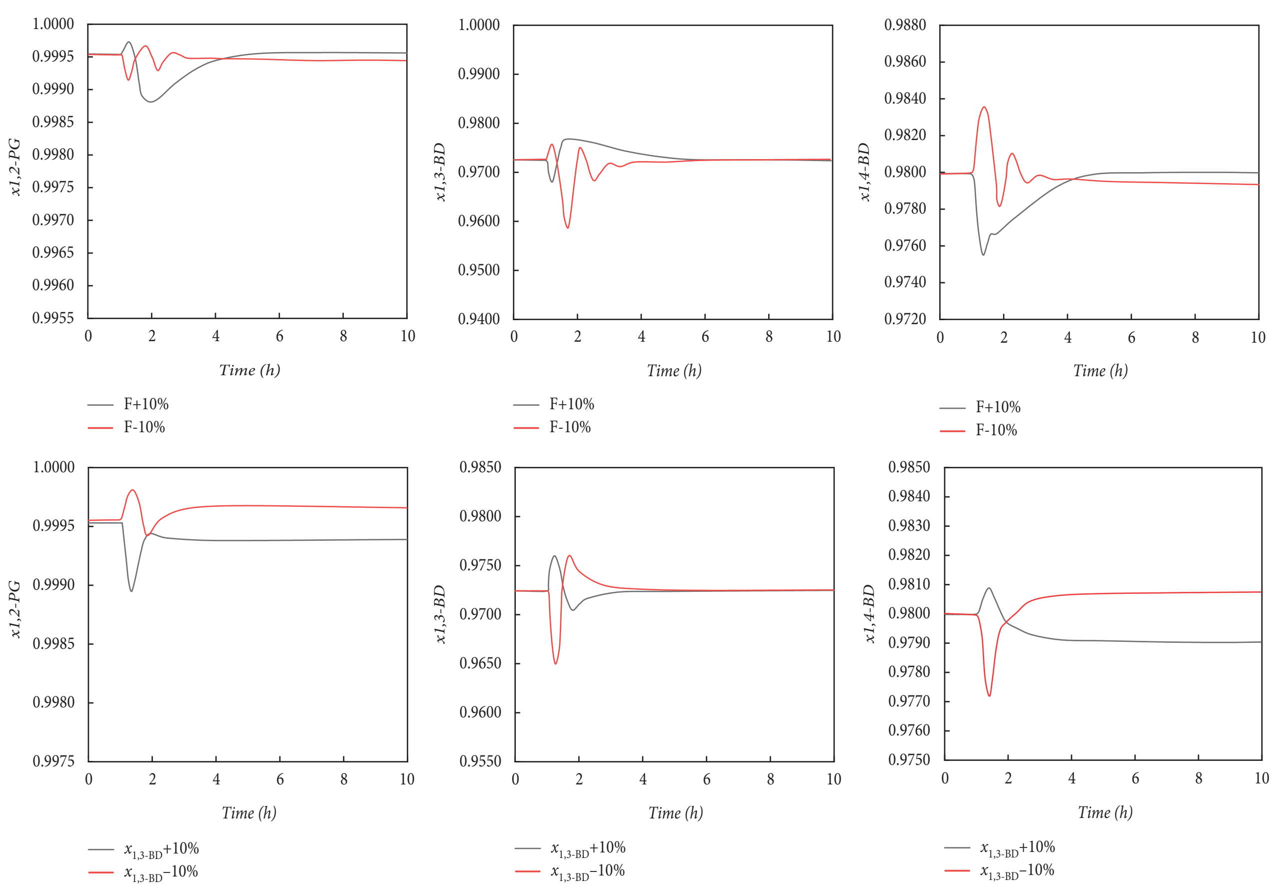

Figure 8: Dynamic responses of CS3 to ±10% feed disturbances.

manipulate RR and an additional flow rate controller was added into side stream control loop. Similar to CS1, stage 5 was taken as reference stage for the rectifying section.

Figure 7 shows the cascade control structure CS3 of DWC. The controller TC1 controlled the temperature at stage 5 by manipulating RR, the cascade loop manipulated S in order to control the purity of 1, 3-BD, and CC3 manipulated Q_R to control the purity of 1, 4-BD. The dead time was 1 min and 3 min for temperature controller and composition controllers, respectively. Table 4 lists the detailed parameters for temperature controller and composition controllers obtained by the relay-feedback test and Tyreus–Luyben tuning method. The other controllers employed same parameters as CS1.

Figure 8 describes the dynamic responses under ±10% feed disturbances, and the product purity could be steady within 4 hr with the same purity as the initial states. The maximum deviations resulted from feed flow rate disturbances in the purity of 1, 2-PG, 1, 3-BD, and 1, 4-BD were 0.07%, 1.44%, and 0.46%, respectively, and the maximum deviations caused by feed composition disturbances were 0.06%, 0.72%, and 0.31%, respectively.

4. Conclusions

In this paper, three types of control structures for DWC were studied by adding ±10% feed disturbances for the ternary glycols (1, 2-PG+ 1, 3-BD+ 1, 4-BD) in a DWC. It showed that CS1 could not deal with the disturbances well while CS2 and CS3 showed a good performance in the face of disturbances. For CS2, three composition controllers were employed to control the purity of products. The dynamic responses showed that the system could get steady within 6 hr and the product purity had small deviations in the face of feed disturbances. For CS3, a temperature controller, two composition controllers, and a flow rate controller were used to control the DWC, in which a composition-flow rate cascade loop was used to control the purity of side stream product. The dynamic responses showed that the system could be steady within 4 hr with small deviations. In comparison with CS2, CS3 had better dynamic responses and all of three products could get steady with smaller deviations, shorter settling time, and smoother responses in most cases.

Data Availability

The data used to support the findings of this study are available from the corresponding author upon request.

Disclosure

The manuscript has been previously presented as poster of AIChE.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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