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Dynamic performance comparison of two configurations of middle vessel batch distillation column for the separation of ethanol/propanol/butanol mixture

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Abstract

This paper deals with Aspen Plus and Aspen Dynamics of the middle vessel batch distillation for the separation of mixtures of ethanol/propanol/butanol. Two configurations of middle vessel batch distillation have been considered, namely, the conventional middle vessel batch distillation (Configuration 1) and the modified middle vessel batch distillation column (Configuration 2). Steady-state simulations have been performed in Aspen Plus and exported to Aspen Dynamics for dynamic simulation. Dynamic studies show that Configuration 1 requires less time than Configuration 2 to obtain more than 95% of the compositions of ethanol, propanol, and butanol. The efficacy of the two controllers is assessed by the performance indices of integral of square error, integral of absolute error, and integral of time-weighted absolute error. Configuration 1 is found to have better performance than Configuration 2.

KEYWORDS

Aspen Dynamics, control structure, middle vessel batch distillation, steady-state simulation

1 | INTRODUCTION

Distillation has become the most prominently used unit operation for separating liquid mixtures in major industries. The two main modes of operation are batch distillation and continuous distillation. Although continuous distillation has long been recognized as much more energy efficient and energy intensive than batch distillation, batch distillation remained as the significant technology due to increased operational flexibility. The flexibility in batch distillation column operation makes it particularly suitable for multipurpose or smaller operations. Manufactures in the chemical industries are an example of these small multiproduct operations, which typically require small quantities of products related to the limited product cycle and fluctuating demand. In particular, the recent research focuses on two key areas: optimal operational control policies for batch distillation columns and the viability of product sequences and optimum column sequences. The most popular type of batch distillation columns is those rectifiers or regular columns for which a larger feed is loaded into the boiler at the base of the rectifier column. Batch strippers are less widely used when feed is introduced into a hold-up tray at the top of the stripping column, and the heavier compounds are collected from the bottom of the column. The batch striper is usually used to separate small quantities of the heavier component from large quantities of light solvents. If a stripper is employed instead of a batch rectifier, the duration of operation optimizes when the product is withdrawn at once. This is contrary to a rectifier, where only after all light components have been boiled off are the products left in the pot.

Nonetheless, the use of batch strippers over a batch rectifier has drawbacks, that is, the highest temperature occurs during the start of the process, and the column is split and often serviced by thermal decomposition reactions and solids in the feed.

Researchers tested a new column concept originally offered by Gilliland and Robinson based on a product sequence feasibility study and optimized column series. A feed is given in a large volume in the middle of the column in this novel configuration. This column includes a stripper as well as a rectifying section in one way.[1] Hasebe et al[2] proposed that the distillation vapor and liquid inlet batch rectifiers be fed into the first column as a stripping section filled into the second batch rectification vessel from the bottom hold up, the rectifier section of the middle vessel. In the middle of a column with a reboiler and a condenser, Davidyan et al[3] suggested the introduction and removal of liquid heat from a holdup tank. The configuration of Hasebe et al[2] is helpful in a plant that also has existing batch rectifiers. Conversely, the configuration of Davidyan et al[3] can be easily applied to a modified continuous distillation column as Barolo et al[4] attempts. This column configuration has been given several names, including the complex batch distillation column and the more definitive middle vessel column. In the last few years, great attention has been paid to the middle vessel batch distillation column (MVBDC).[5]A new algorithm has been developed for product sequences for the batch distillation column of a mixture containing any number of components. This can be done in accordance with the temperature of pure components, azeotropic compositions, and azeotropes. The pressure swing batch distillation for the separation of dichloromethane/methanol binary azeotropy mixture by the AspenTech simulation platform has been implemented with a cascade composition rate structure.[6]

In the past couple of years, the study of the MVBDC has received considerable scientific attention.[7-9] Luyben[10] performed Aspen dynamic simulation of conventional MVBDC. Rao and Barik[11] discussed the mathematical modeling, simulation, and control of modified middle vessel batch distillation column. An MVBDC has been used to separate a mixture of methyl formate–methanol–water mixture. Zhu et al[12] showed that the temperature control structure can successfully separate the ternary system. In contrast with the composition control structure, two temperature control systems, one with a conventional temperature control structure and the other with a high-selector temperature control structure, show better control outputs.[13]

The middle-vessel configuration compared with conventional batch processes reduces mixing and saves energy. In this work, a study has been carried out on two configurations of MVBDC, namely, conventional MVBDC (Configuration 1) and modified MVBDC (Configuration 2). In Configuration 1, the vapor from the stripping section goes directly into the sump of the rectification section. In contrast, in Configuration 2, the vapor from the stripping section passes into the middle vessel and then enters the rectification section sump to separate the ethanol/propanol/butanol ternary mixtures. The middle vessel in Configuration 2 serves as an equilibrium stage like the other trays, whereas in Configuration 1, it is only a storage vessel. In recent years, much research has been reported on these new columns. However, there are no reports of steady-state and dynamic studies of middle vessel batch distillation for the separation of ethanol/propanol/butanol mixtures. The control structures must always be adequately evaluated in order to make sure that process operations are efficient, as a good control structure can not only simplify the separation process but also ensure that the products are highly pure. Furthermore, the two control structures have been investigated using Aspen Dynamics studies to evaluate the superiority of the above-mentioned configurations.

2 | SIMULATION STUDIES

2.1 | Steady-state simulation condition and method

In this work, ethanol/propanol/butanol mixtures were separated by the middle vessel batch distillation column using the Aspen Plus software. First, models were built in the graphical user interface. RadFrac was used as the stripper and rectifier. A flash drum was used as the middle vessel. An attempt was made to extract the low, medium, and high boiling fractions from the rectifier, flash drum, and stripper, respectively. An Aspen flow sheet diagram for two configurations of MVBDC is shown in Figures 1 and 2. A nonrandom two-liquid method has been chosen as a thermodynamic model for the solution of the model equations. The stages are numbered from top to bottom in both the sections. The number of stages in the rectifier and stripper is 14 each. The feed mixture is fed into the sump of the stripper at 10 kmol/hr with compositions of 40% ethanol, 40% propanol, and 20% butanol. The molar flow rate of vapor stream that is coming out from the top of the stripper is fixed at 5 kmol/hr for both configurations. In the case of Configuration 1, this vapor stream goes directly into the sump of the rectifier, but in the Configuration 2, it enters the sump of the rectifier through the middle vessel. At the end of the steady-state simulation, the compositions of 100, 99, and

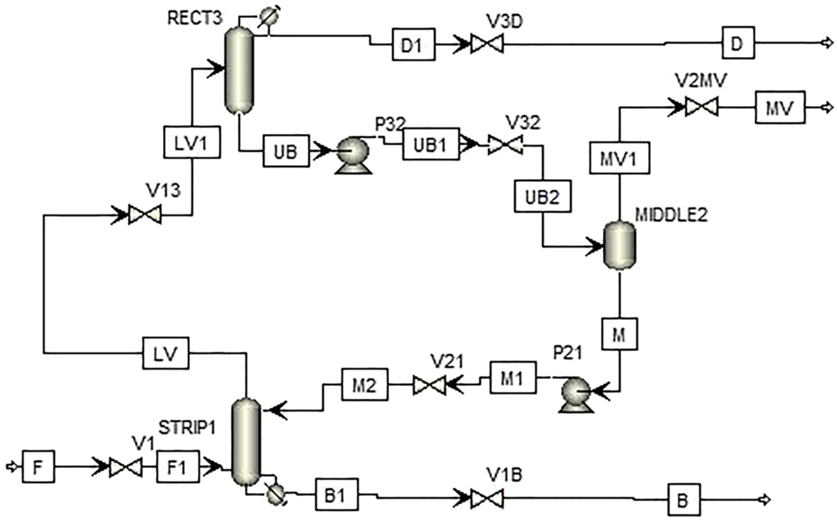

FIGURE 1 Aspen plus flow sheet of configuration 1

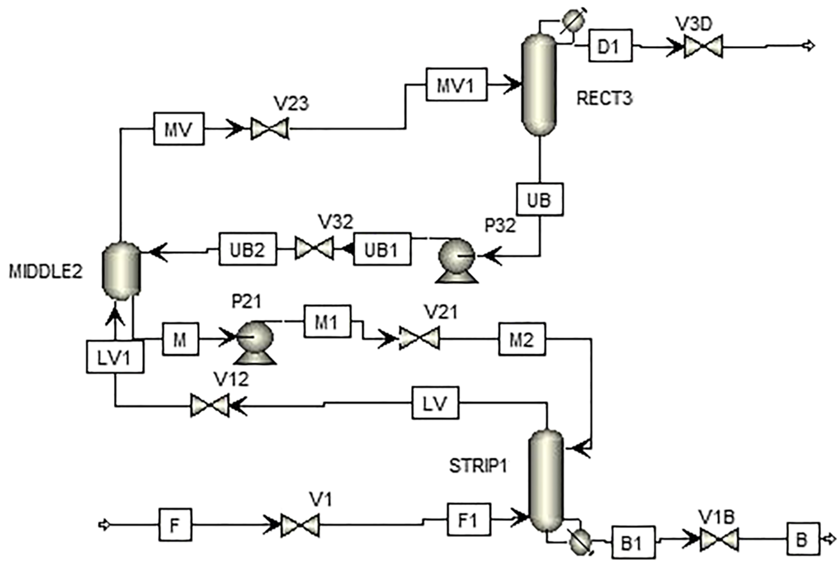

FIGURE 2 Aspen plus flow sheet of configuration 2

40 mol% of ethanol are obtained at reflux drum of rectifier, middle vessel, and sump of the stripper, respectively. The stream results after Aspen Plus steady-state simulation are given in Table 1.

The reflux drum, middle vessel, and the sump of the stripper principally act as storage vessels for ethanol, propanol, and butanol, respectively, at the end of batch simulation. Before exporting into the Aspen Dynamics, these vessels are properly sized in order to store the respective components. The sump of the stripper is sized with 2-m diameter and 4-m length, giving the volume of 12.5 m^3 and initial specification of 0.05 total liquid volume fractions, which is enough to store the batch feed of 120 kmol with composition 40 mol% ethanol, 40 mol% propanol, and 20 mol% butanol. Keeping the view on dynamic fluctuations in the holdups of the middle vessel, reflux drum, and sump of the rectifier, these are sized with 2-m diameter and 4-m height (volume 12.5 m^3), 1.7-m diameter and 3.4-m length (volume 7.7 m^3), and 1.5-m diameter and 3-m length (volume 5.3 m^3), and 0.05 initial liquid volume fraction, respectively.

2.2 | Dynamic simulation condition and method

The steady-state information obtained in Aspen Plus can be used in Aspen Dynamics. However, there are two different programs with separate files. The Aspen Plus file was saved with the filename as filename.apw, and a backup file with the filename as filename.bkp was also created. The latter is now available for upgrading to new Aspen Plus versions. The Aspen Plus knowledge is "exported" to Aspen Dynamics by creating two more

TABLE 1 Steady state stream results after Aspen plus simulation

	Feed		Bottom		Middle		Distillate	
	C1	C2	C1	C2	C1	C2	C1	C2
Total flow ate (kmol/hr)	**10**	**10**	**9.895**	**9.9**	**4.895**	**4.9**	**0.1**	**0.1**
Component flow rate (kmol/hr)								
Ethanol	4	4	3.895	3.9	4.894	4.9	0.1	0.1
Propanol	4	4	4	4	4.02×10^{-4}	4.49×10^{-6}	2.71×10^{-9}	9.60×10^{-12}
Butanol	2	2	2	2	8.06×10^{-9}	9.87×10^{-8}	8.27×10^{-19}	3.44×10^{-18}
Mole fraction (x)								
Ethanol	0.4	0.4	0.394	0.394	0.999	0.999	1	1
Propanol	0.4	0.4	0.404	0.404	8.21×10^{-5}	9.18×10^{-7}	2.71×10^{-8}	9.60×10^{-11}
Butanol	0.2	0.2	0.202	0.202	1.64×10^{-9}	2.01×10^{-8}	8.27×10^{-18}	3.44×10^{-17}

Abbreviations: C1, Configuration 1; C2, Configuration 2.

files. The first one is an Aspen Dynamics file labeled filename.dynf. After exporting into the Aspen Dynamics, first, all the default controllers are removed. The valves, namely, V1, V1B, V2MV, and V3D (shown in Figures 1 and 2), should be closed by setting valve position to 0% in order to convert the continuous distillation to batch distillation. Now, the system is fully closed middle vessel batch distillation, and the feed of 120 kmol is in the sump of the stripper.

The startup operation of the distillation columns was analyzed by Barolo et al[14] and Elgue et al.[15] The startup operation of the middle vessel batch distillation was also broadly discussed by Gruetzmann and Fieg.[16] The lower sump of the stripper is filled with the ethanol/propanol/butanol mixture to create the liquid level. The steam is supplied to the reboiler to heat the liquid. The liquid gets heated, and it goes up when it reaches the bubble point temperature of the mixture. In Configuration 1, the rising vapor leaves the top of the stripper and goes to the condenser and gets condensed into liquid. The liquid starts to fill the reflux drum. Once the sufficient liquid level is attained for pump Net Positive Suction Head requirements, the reflux begins to flow down to the rectifier. Although the liquid is going down to the rectifier, it comes in contact with the vapor, and hence, the separation takes place. The liquid starts to fill the sump of the rectifier, and after pump Net Positive Suction Head requirements are achieved, the valve V32 is opened to allow liquid into the middle vessel. The levels of the reflux drum and the sump of the rectifier are maintained at low levels. The same operation is being followed for Configuration 2. The only difference is that the vapor from the top of the stripper goes to the condenser through the middle vessel. The holdup in the middle vessel starts to build up, and when the liquid level is appropriately enough, the liquid is pumped into the top of the stripper through the valve V21. The liquid starts flowing down the stripper. The vapor goes up, and the liquid comes down.

For a constant reboiler heat duty, the holdup in the sump of the lower column decreases with time, and gradually, it becomes empty. So, it is necessary to maintain the temperature of the sump of the stripper at nominal value instead of the reboiler duty. Alternatively, the level in the reboiler can also be maintained at a constant value. Hence, two control structures have been studied. The structure that includes reboiler temperature controller at the lower column along with three level controller at the upper column reflux drum, upper column sump, and middle vessel is termed as the temperature control structure, and the structure that includes four level controls at the upper column reflux drum, upper column sump, middle vessel, and lower column sump is named as the level control structure.

3 | RESULTS AND DISCUSSION

A dynamic comparison study has been carried out for Configurations 1 and 2 for both the control structure (temperature control structure and level control structure), and the results are obtained.

3.1 | Comparisons of configurations for the temperature control structure

This control structure consists of four controllers at the reflux drum of a rectifier, at the sump of a rectifier, at the middle vessel, and at the sump of a stripper. There are three level controllers among the four controllers and one temperature controller. The three level controllers are installed at the reflux drum of the rectifier, at the sump of the rectifier, and at the middle vessel, and the temperature controller is placed at the sump of the stripper. It can be seen from Figures 3 and 4 that the levels at the reflux drum of the rectifier, at the sump of the rectifier, and at the middle vessel are maintained by manipulating the reflux flow rate, percentage of a valve (V32) opening, and percentage of a valve (V21) opening, respectively. The temperature at the sump of the stripper is maintained by manipulating the reboiler heat duty. The dynamic responses of the composition, temperature, and holdups are obtained and analyzed for both the configurations. Figures 5 and 6 gives the composition profiles of temperature control structure for Configurations 1 and 2, respectively. From Figures 5 and 6, it is observed from both the configurations that ethanol and butanol, which are light and heavy fractions, can be obtained simultaneously from the top and bottom of the column, and the intermediate boiling fraction, that is, propanol, accumulates in the middle vessel. It is clearly seen form Figure 5 that Configuration 1 requires less than 10 hr to obtain more than 95% of ethanol, propanol butanol at rectifier, middle vessel, and stripper. However, Configuration 2 takes twice as much time, that is, the time required to

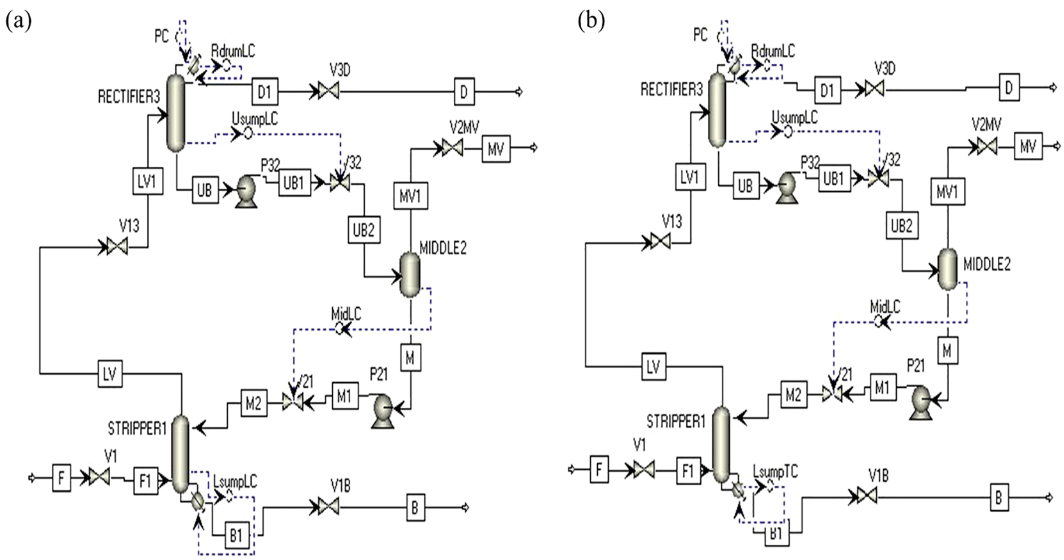

FIGURE 3 Aspen dynamics flow sheet of configuration 1. (a) Level control structure and (b) temperature control structure

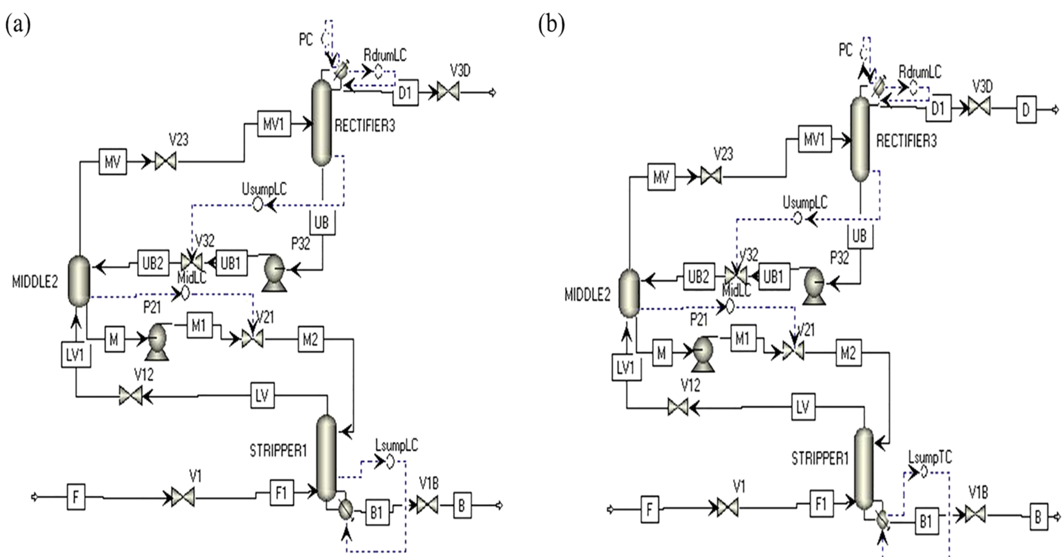

FIGURE 4 Aspen dynamics flow sheet of configuration 2. (a) Level control structure and (b) temperature control structure

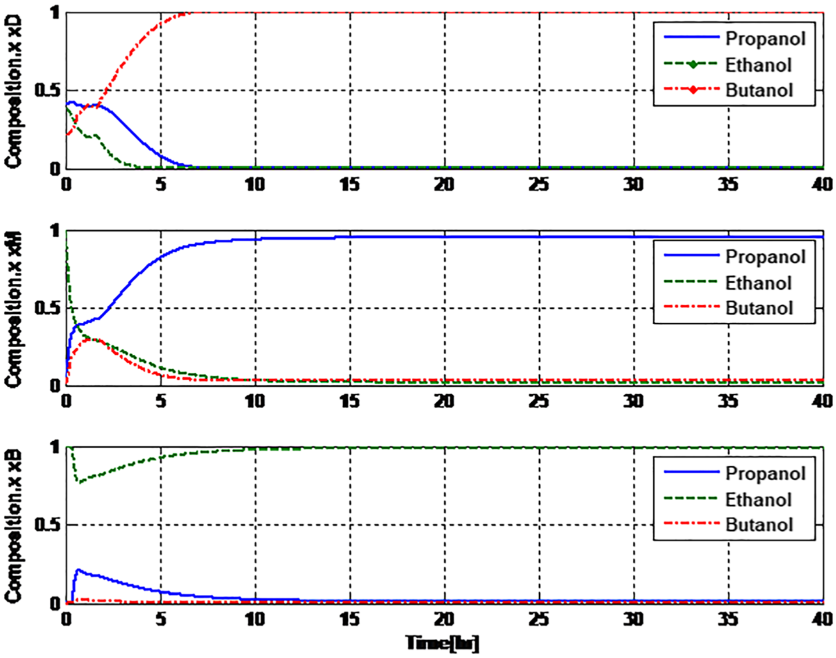

FIGURE 5 Composition profiles of configuration 1 for temperature control structure

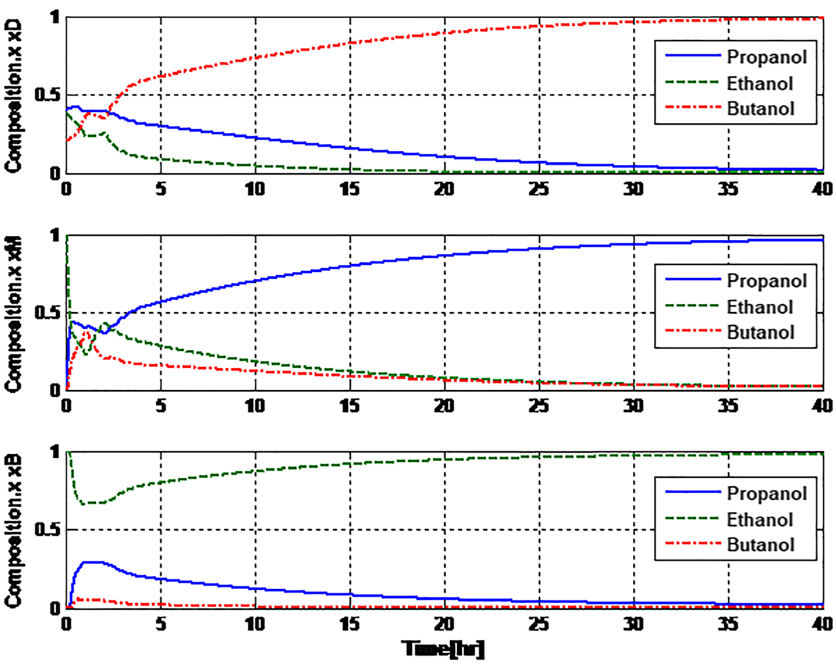

FIGURE 6 Composition profiles of configuration 2 for temperature control structure

reach steady state as Configuration 1 to achieve more than 95% composition of ethanol, propanol, and butanol at the respective sections. The temperature profiles at reflux drum, middle vessel, and lower sump are shown in Figure 7. As can be seen from Figure 7 that the steady-state time for Configuration 1 is less compared with Configuration 2. Holdup profiles at the reflux drum of the rectifier, at the sump of the rectifier, and at the middle vessel and sump of the stripper have also been analyzed for the configurations and is given in Figure 8. The closed-loop response resulted from Configuration 1 has less oscillations than Configuration 2 as shown in Figure 8.

3.2 | Comparisons of configurations for the level control structure

This control structure consists of four level controllers at the reflux drum of the rectifier, at the sump of the

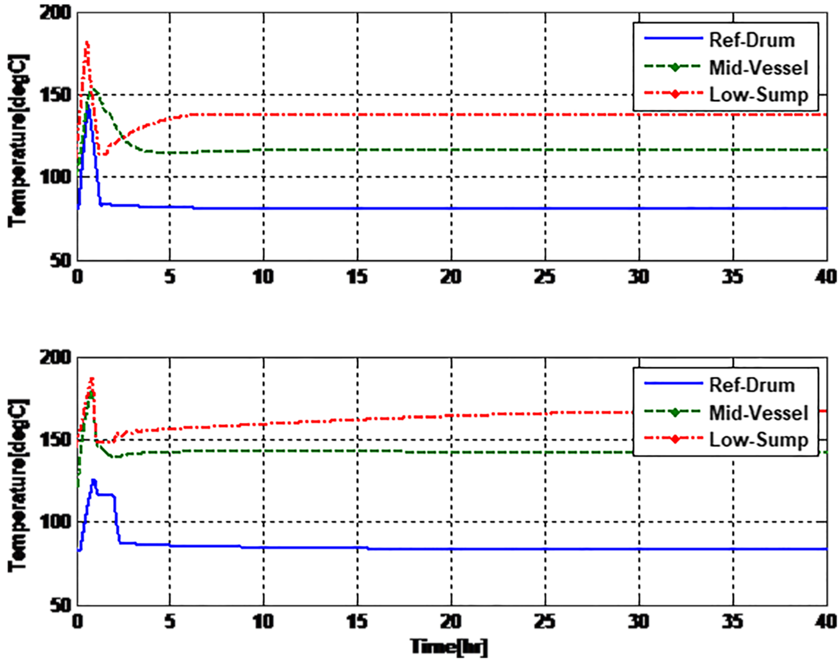

FIGURE 7 Temperature profiles of configurations 1 (top) and 2 (bottom) for temperature control structure

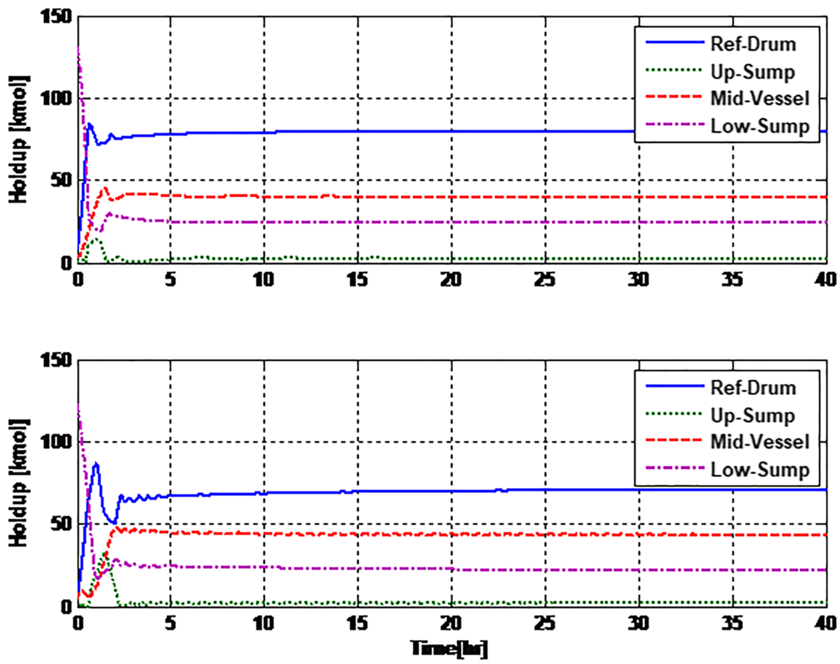

FIGURE 8 Holdups of configurations 1 (top) and 2 (bottom) for temperature control structure

rectifier, at the middle vessel, and at the sump of the stripper. The levels at the reflux drum of the rectifier, sump of the rectifier, middle vessel, and sump of stripper are maintained by manipulating the reflux flow rate, percentage of valve (V32) opening, percentage of valve (V21) opening, and reboiler heat duty, respectively. The dynamic responses of the composition, temperature, and holdups are obtained and analyzed for both the configurations. Closed-loop performance of the level control structure for both the configurations has been carried out and shown in Figures 9 and 10. The same observations have also been seen in the level control structure. Figures 9 and 10 show that ethanol and butanol, which are light and heavy fractions, have been obtained simultaneously from the top and bottom of the column and that the intermediate boiling fraction, that is, propanol, accumulates in the middle vessel. More than 95% of the compositions of ethanol, propanol, and butanol are achieved from Configuration 1 in less than 10 hr, whereas Configuration 2 takes more than 20 hr. The simulation studies

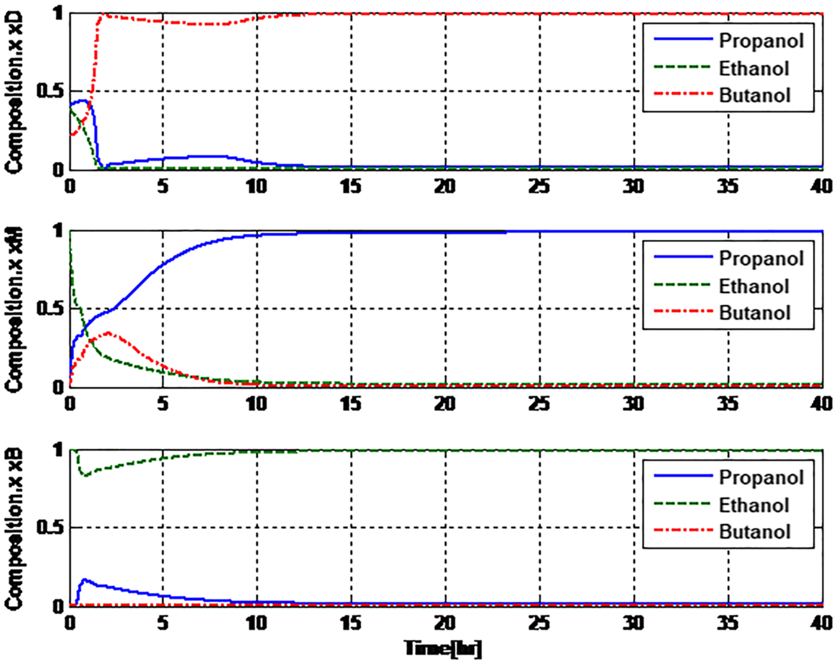

FIGURE 9 Composition profiles of configuration 1 for level control structure

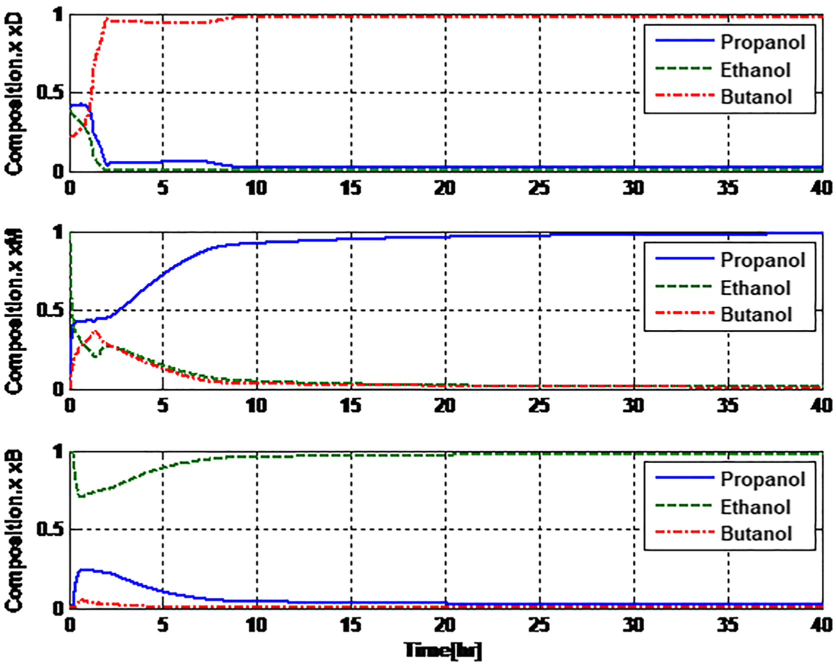

FIGURE 10 Composition profiles of configuration 2 for level control structure

have been performed to obtain a closed-loop response of the temperature profiles at the reflux drum, middle vessel, and lower sump, and the obtained results are shown in Figure 11. In contrast to Configuration 2, the time required to reach a steady state for Configuration 1 is also lower in this control structure. Figure 12 shows the holdup profiles at the reflux drum of the rectifier, sump of rectifier, middle vessel, and sump of the stripper. The dynamic response of the holdups at the reflux drum of the rectifier, sump of the rectifier, middle vessel, and sump of the stripper resulted from Configuration 1, which has lesser oscillations compared with Configuration 2.

3.3 | Controller performance of the two control structure

The rigorous closed-loop simulations have been conducted to evaluate the superiority between the two configurations. The closed-loop servo response of the level

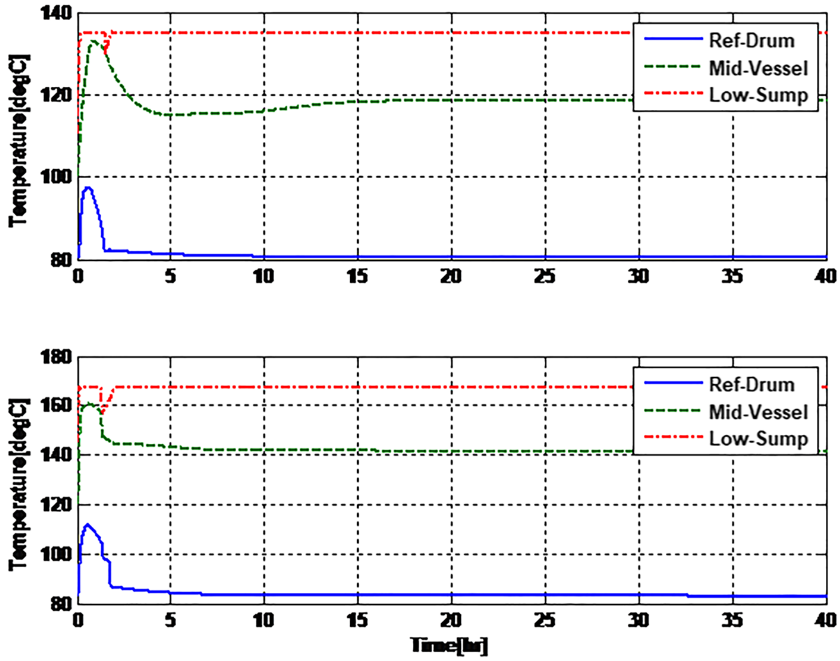

FIGURE 11 Temperature profiles of configurations 1 (top) and 2 (bottom) for level control structure

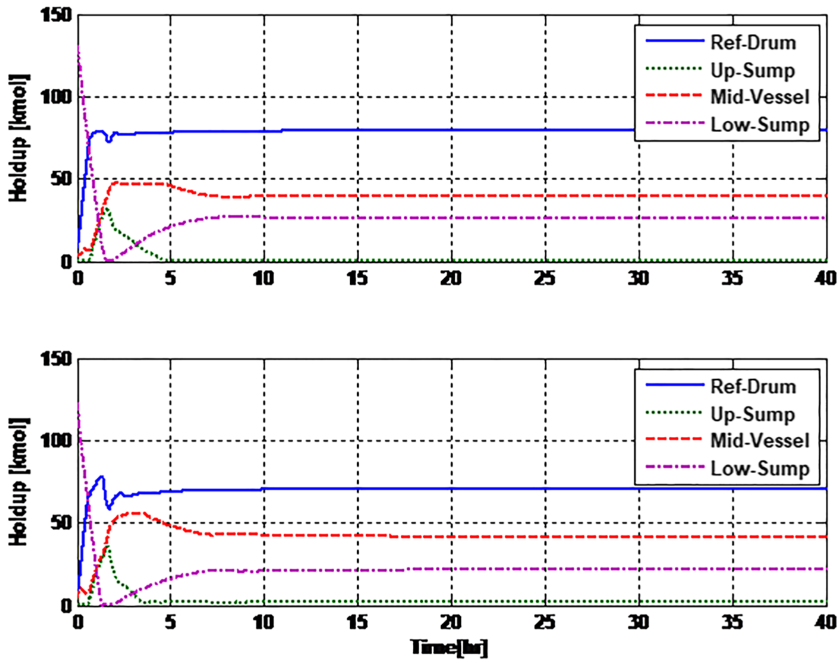

FIGURE 12 Holdups of configurations 1 (top) and 2 (bottom) for level control structure

control structure for Configurations 1 and 2 is shown in Figures 13 and 14, respectively. For a level controller, set point is the required level and process variable is the transient liquid level in the corresponding sections such as reflux drum and sump. From the closed-loop performance of Configuration 1, it can be seen that all the levels reach set point except the level at the sump of the rectifier. When compared with Configuration 2, it can be observed that all the closed-loop levels obtained from Configuration 2 track the set point, whereas the level at the sump of the rectifier obtained from Configuration 1 fluctuates. The closed-loop response obtained from the temperature control structure of both the configurations has been shown in Figures 15 and 16. Figure 15 shows the closed-loop response of the temperature control structure for Configuration 1. The transient response of temperature at the lower sump of the stripper and the transient response of the level at the middle vessel, at the reflux drum, and at the sump of the rectifier attain the set point. Figure 16 shows the closed-loop response of the

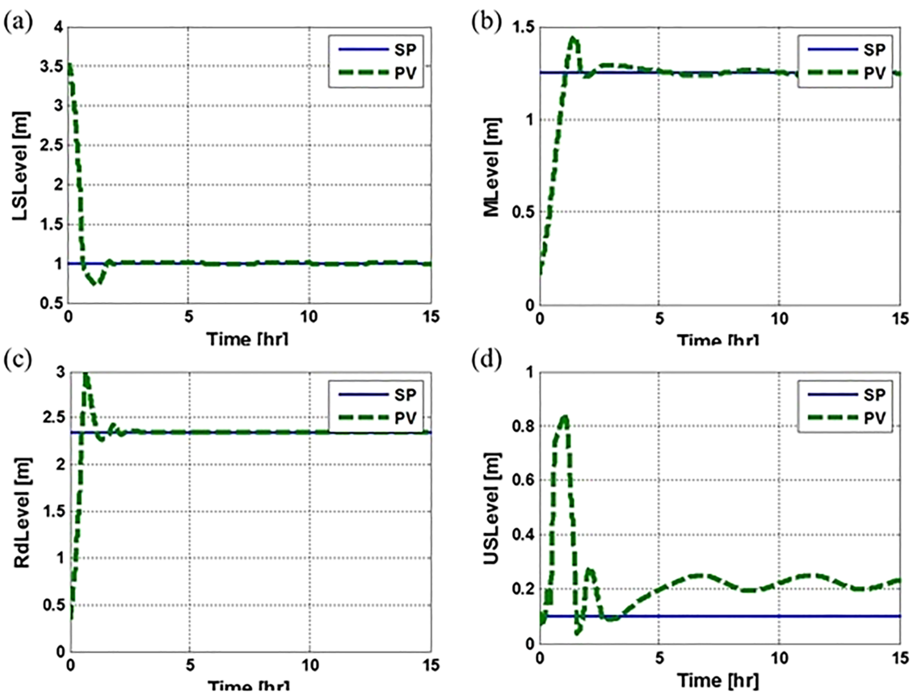

FIGURE 13 Closed-loop servo response of the level controller structure. (a) Level at sump of stripper, (b) level at middle vessel, (c) level at reflux drum, and (d) level at sump of rectifier for configuration 1. LS, level at sump; ML, Level at middle vessel; PV, process variable; SP, set point

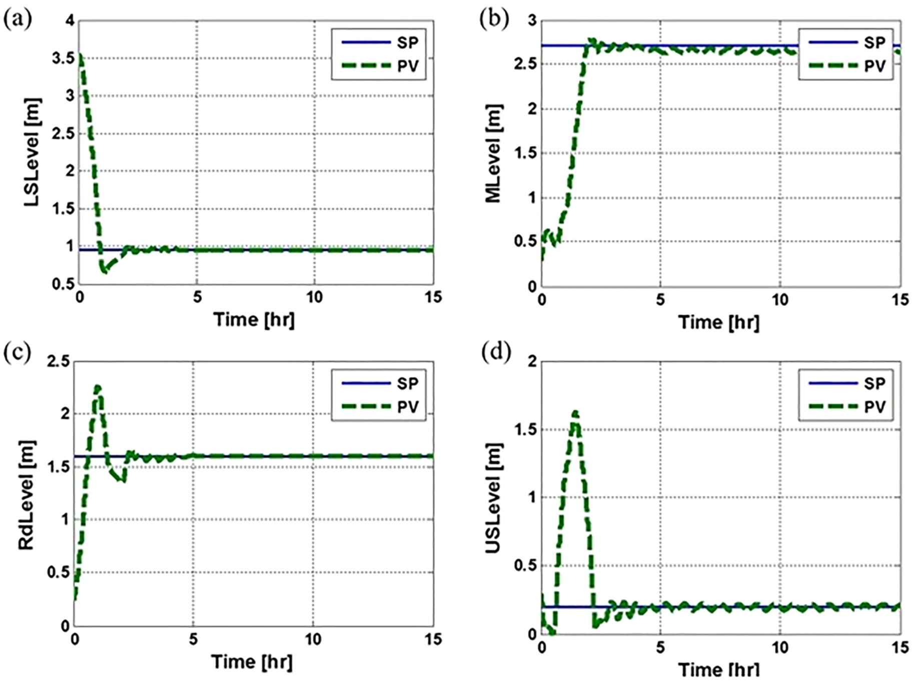

FIGURE 14 Closed-loop servo response of the level controller structure. (a) Level at sump of stripper, (b) level at middle vessel, (c) level at reflux drum, and (d) level at sump of rectifier for configuration 2. LS, level at sump; ML, middle vessel; PV, process variable; SP, set point

temperature control structure for Configuration 2. From Figures 15 and 16, it can be seen that the temperature control of Configuration 2 works better.

The quantitative analysis in terms of time integral error such as integral of absolute error (IAE), integral of time weighted absolute error (ITAE), and integral of square error (ISE) is given in Table 2. The controller performances are evaluated by IAE, ITAE, and ISE. Table 2 gives the controller performance of the temperature control structure for both the configurations. From Table 2, the following inferences can be brought. From Table 2, it can clearly be inferred that the IAE values obtained from all the controllers of Configuration 1 are lesser as compared with Configuration 2.

For the level controller installed at the reflux drum of a rectifier, IAE values are reduced by 9% from

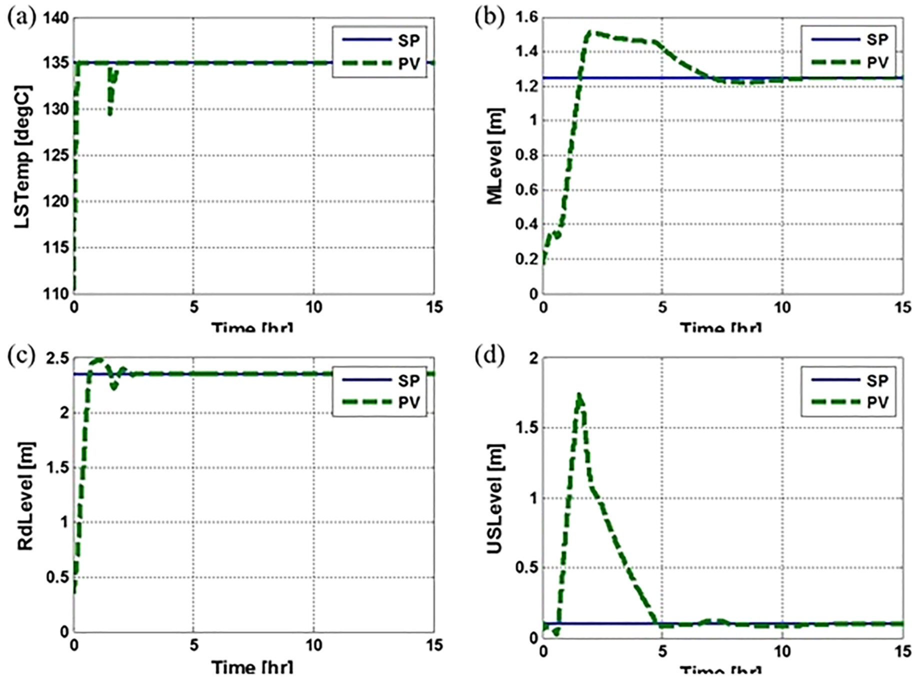

FIGURE 15 Closed-loop servo response of the temperature controller structure. (a)temperature at sump of stripper, (b) level at middle vessel, (c) level at reflux drum, and (d) level at sump of rectifier for configuration 1. LS, level at sump; ML, middle vessel; PV, process variable; SP, set point

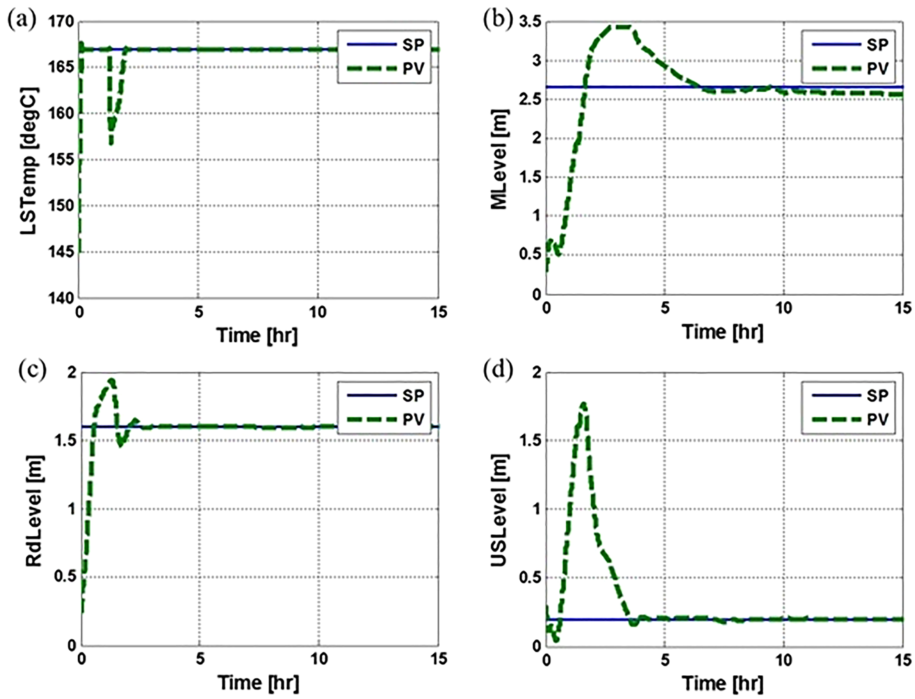

FIGURE 16 Closed-loop servo response of the temperature controller structure. (a) Temperature at sump of stripper, (b) level at middle vessel, (c) level at reflux drum, and (d) level at sump of rectifier for configuration 2. LS, level at sump; ML, middle vessel; PV, process variable; SP, set point

TABLE 2 Controller performance of temperature control structure for both the configurations

	C1	C2	C1	C2	C1	C2	C1	C2
Error Values	**LC1**		**LC2**		**LC3**		**TC1**	
IAE	148.95	161.57	213.13	273.80	141.38	553.62	214.12	275.35
ITAE	62.33	149.35	772.06	462.20	142.51	644.66	80.93	140.79
ISE	175.20	106.62	72.66	245.45	88.35	964.60	379.27	466.79

Abbreviations: IAE, integral of absolute error; ISE, integral of square error; ITAE, integral of time weighted absolute error; LC1, level controller at reflux drum (rectifier); LC2, level controller at sump (rectifier); LC3, level controller at middle vessel; TC1, temperature controller at sump (stripper).

TABLE 3 Controller performance of level control structure for both the configurations

Variable	LC1 C1	LC1 C2	LC2 C1	LC2 C2	LC3 C1	LC3 C2	LC4 C1	LC4 C2
IAE	141.86	116.86	466.73	338.65	336.46	769.05	480.89	851.69
ITAE	58.02	91.55	1040.2	604.29	713.21	1577.5	225.14	974.62
ISE	174.02	75.56	441.38	325.99	179.49	916.48	6136.1	7740.50

Abbreviations: IAE, integral of absolute error; ISE, integral of square error; ITAE, integral of time weighted absolute error; LC1, level controller at reflux drum (rectifier); LC2, level controller at sump (rectifier); LC3, level controller at middle vessel; LC4, level controller at sump (stripper).

Configuration 1 (C2) to Configuration 2 (C1), and ITAE values are reduced by 140% from C2 to C1. For the level controller installed at the sump of the rectifier, IAE values are reduced by 28% from C2 to C1, and ISE values are reduced by 140% from C2 to C1. The level controller installed at the middle vessel produces comparatively larger errors for C2 compared with C1. Using this controller, a 291% reduction in IAE, a 352% reduction in ITAE, and 991% reduction in ISE are achieved by C1 when compared with C2. The temperature controller, which is installed at the sump of the stripper, produces lower values of IAE, ITAE, and ISE. There is a 28, 73, and 23 reduction in IAE, ITAE, and ISE for C1 compared with C2. It is therefore clear from Table 2 that Configuration 1 shows better performance in terms of time integral error.

A similar analysis has been performed for the level control structure (Table 3) for C1 and C2. The level controller installed at the middle vessel produces comparatively larger errors for C2 compared with C1. Using this controller, 128% reduction in IAE, 121% reduction in ITAE, and 411% reduction in ISE are achieved by C1 when compared with C2. A level controller that is installed at the sump of the stripper produces lower values of IAE, ITAE, and ISE. There is a 77%, 332%, and 26% reduction in IAE, ITAE, and ISE for C1 compared with C2. From these analyses, it can be said that Configuration 1 shows better performance in terms of time integral error compared with Configuration 2.

4 | CONCLUSIONS

This paper investigates the steady-state and dynamic simulations of two configurations of the MVBDC for separating a mixture of ethanol, propanol, and butanol. In one configuration, the middle vessel was treated as a storage tank, and in the other case, the middle vessel serves as an equilibrium stage. Different control structures, such as temperature control structure and level control structure, were also being studied for both configurations. The dynamic results showed that more than 95% of ethanol, propanol, and butanol compositions were obtained in less than 10 hr for Configuration 1, whereas Configuration 2 requires more than 20 hr for both control structures. The observations from dynamic simulation studies of temperature control structure suggested that Configuration 1 takes a larger time to obtain higher purity when compared with Configuration 2. Closed-loop responses obtained from C1 had less oscillations and better set point tracking ability. The above-mentioned claims were confirmed with the quantitative analysis, that is, using time integral errors. It is therefore recommended that Configuration 1 be used over Configuration 2.

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