Effect of Feed Composition on the Selection of Control Structures for High-Purity Binary Distillation

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This paper discusses the selection of an effective control structure for a binary distillation column producing high-purity products. Results show that this selection depends on the feed composition. If the concentration of the light component is *large*, the reflux ratio is small. Control of a single appropriate tray temperature by manipulating the reboiler heat input and using a fixed feed-to-reflux ratio provides effective control for both feed-rate and feed-composition disturbances. The reflux-drum level is controlled by the distillate flow rate. For *intermediate* concentrations of the light component and for high-purity products, this study shows that a two-temperature control structure with reflux and reboiler heat input manipulated is required to handle feed-composition changes. *Small* concentrations of the light component yield small distillate flow rates and high reflux ratios. Conventional distillation control wisdom advises that the reflux-drum level should be controlled by the reflux flow rate when the reflux ratio is larger than ∼2. A control structure is frequently recommended in which the flow rate of the distillate is ratioed to the reflux. However, in many columns, a constant reflux-ratio strategy is not as effective as a constant reflux-to-feed strategy for maintaining product purity at both ends of the column in the face of feed-composition disturbances when a single tray temperature is controlled. An alternative control structure is proposed in this paper that achieves the preferred constant reflux-to-feed strategy by controlling the reflux-drum level with reboiler heat input and manipulating the small distillate flow rate to control a tray temperature.

1. Introduction

The distillation control literature is one of the most extensive in the area of process control. The last half of the 20th century produced thousands of papers and several books on the subject. The rate of publications during the past decade has slackened significantly because of the de-emphasis on research in distillation by the funding agencies, which drives most academic studies. However, distillation remains the primary separation method in the petroleum and chemical industries, and its practical importance is unquestionable.

There are many different types of distillation columns and many different types of control structures. The selection of the "best" control structure is not as simple as some papers claim. Factors that influence the selection include volatilities, product purities, reflux ratio, column pressure, cost of energy, and column size.

This paper explores another factor that impacts the selection of an effective control structure: the composition of the feed. We consider a binary system, with the specific example of the methanol/water separation. This system is important in itself, but it is also typical of many binary separations involving fairly high-purity products. In some processes, the concentration of the light component in the feed is small (<10 mol %). In other processes, it is large (>90 mol %). Other processes have intermediate feed compositions.

A large concentration of the light component in the feed corresponds to moderate reflux ratios, unless relative volatilities are quite small, because the distillate flow rate is large. This means that the reflux-drum level can be controlled by either the reflux or the distillate. A control structure often recommended for low to modest reflux ratio columns is the following:

1. Control the reflux-drum level by manipulating the distillate.
2. Control an appropriate tray temperature by manipulating the reboiler heat input.
3. Control the reflux-to-feed ratio (R/F) by measuring the flow rate of the feed, multiplying this signal by the desired reflux-to-feed ratio, and setting the setpoint of a remote-set flow controller on the reflux.
4. Control the base level by manipulating the bottoms flow rate.
5. Control the pressure by manipulating the condenser heat removal.

A small concentration of the light component in the feed means large reflux ratios because the distillate flow rate is small. Conventional distillation control heuristics advise that the reflux-drum level should be controlled by the reflux flow rate when the reflux ratio is larger than ∼2 or 3. Therefore, a control structure often recommended for high reflux ratio columns is the following:

1. Control the reflux-drum level by manipulating the reflux.
2. Control an appropriate tray temperature by manipulating the reboiler heat input.
3. Control the reflux ratio by measuring the flow rate of the reflux, multiplying this signal by the reciprocal of the desired reflux ratio, and setting the setpoint of a remote-set flow controller on the distillate.
4. Control the base level by manipulating the bottoms flow rate.

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5. Control the pressure by manipulating the condenser heat removal.

When the control structure features the control of a single temperature, the remaining control degree of freedom must be specified. The two most common alternatives are constant reflux ratio and constant reflux-to-feed ratio. They are both equally effective in handling feed flow rate disturbances. In many separations, the constant reflux-to-feed structure (R/F) provides better steady-state product purities for changes in feed composition than the constant reflux ratio structure (RR)[1]. This is demonstrated later in this paper for the specific chemical components used in the example.

The control of two temperatures instead of a single temperature is sometimes discussed in the literature, but it is not clear when this more complex control structure is really required. The presence of the interaction between the two temperature loops makes controller tuning more difficult. However, dual-temperature control has the potential advantage of maintaining the purities of both the distillate and the bottoms products closer to the desired specifications.

2. Process Studied

The binary distillation of methanol/water is used as a numerical example in this paper, but the results should be applicable to many binary separations. The separation of methanol from water is a very common and important distillation system. Methanol is usually produced from synthesis gas, a mixture of hydrogen, carbon monoxide, and carbon dioxide, which typically comes from a steam/methanol reforming process. Water is also produced in the methanol reactor and must be removed.

There has been an enormous interest in the "hydrogen economy" in recent years. From a purely technical perspective, much of this appears to be hype. A "methanol economy" seems to be much more realistic technically, since synthesis gas can be produced by the partial oxidation of any combustible hydrocarbon, including renewable sources such as trees and agricultural byproducts. Methanol is a convenient fuel for automobiles, as demonstrated by its use in World War II for tank fuel. The future uses of methanol may be much more extensive than present consumption. In any event, the methanol/water separation provides a typical example of a binary high-purity separation problem.

In the following sections, distillation columns are designed for a range of feed compositions: 10, 20, 40, 60, 80, and 90 mol % methanol. Each column is optimized in terms of steady-state economics, yielding columns with different numbers of trays, different feed trays, and different reflux ratios. Then the dynamic control of each is explored.

The simulations use the rigorous nonlinear models in the commercial simulation tools Aspen Plus and Aspen Dynamics. The van Laar physical property package is used because of its known ability to closely match experimental methanol/water vapor−liquid equilibrium data. All columns operate at atmospheric pressure with a 0.0068 atm pressure drop per tray. The feed flow rate is 1 kmol/s. The Aspen tray numbering notation is used (stages numbered from the reflux drum down to the reboiler). Total condensers, partial reboilers, and theoretical trays are used. We consider in this paper a column producing high purity products at both ends.

Table 1. Basis of Economics

condensers:
heat-transfer coefficient = 0.852 kW/K·m^2
differential temperature = 13.9 K
capital cost = 7 296(area, m^2)$^{0.65}$
Reboilers:
heat-transfer coefficient = 0.568 kW/K·m^2
differential temperature = 34.8 K
capital cost = 7 296(area, m^2)$^{0.65}$
column vessel capital cost = 17 640(ID, m)$^{1.066}$(L, m)$^{0.802}$
L = NT(1.2)(0.61 m/tray)
energy cost = \$4.7 per 10^6 kJ
TAC = [(capital cost)/(payback period)] + energy cost
payback period = 3 years

Table 2. Design Parameters and Economic Results

feed comp. (mf MeOH)	0.10	0.20	0.4	0.6	0.8	0.9
total stages	42	37	32	32	37	32
feed stage	13	14	16	19	25	21
RR	4.11	2.04	1.00	0.645	0.456	0.396
ID (m)	3.08	3.42	3.98	4.45	4.83	5.06
Q_R (MW)	22.1	25.4	31.6	37.6	43.4	46.4
Q_C (MW)	17.8	21.3	28.1	34.6	40.9	44.1
AR (m^2)	1120	1280	1600	1900	2190	2340
AC (m^2)	1500	1800	2370	2920	3450	3720
shell cost (10^6 \$)	0.879	0.881	0.916	1.83	1.27	1.18
HX cost (10^6 \$)	1.55	1.72	2.02	2.29	2.54	2.66
energy cost (10^6 \$/y)	3.28	3.76	4.69	5.58	6.43	6.88
capital (10^6 \$)	2.42	2.60	2.94	3.32	3.81	3.84
TAC (10^6 \$/y)	4.09	4.62	5.66	6.69	7.70	8.16

The purities of distillate and bottoms streams are set at 99.9 mol %. The Aspen "Design Spec-Vary" feature is used to adjust the distillate-to-feed ratio and the reflux ratio to achieve these purities.

3. Steady-State Design

The economic objective function is the minimum total annual cost (TAC), which includes both energy and capital costs. Table 1 gives the economic parameters. Column diameters are calculated by the Aspen tray sizing procedure. Column height is calculated assuming a 0.61-m spacing per tray and 20% additional shell length for base, feed, and overhead volume.

For each feed composition, the total number of stages is varied until TAC is minimized. For each selection of total stages, the feed stage that minimizes the reboiler heat input is determined. Table 2 gives details of all the designs. Figure 1 shows how the feed composition affects some of the important variables of the column design.

The total number of trays initially decreases as feed composition z (mole fraction of methanol) increases, but it eventually begins to increase. The reflux ratio decreases as z increases. All other parameters increase as the feed becomes richer in methanol, because more material must be vaporized and taken overhead as the distillate product.

Figure 2 gives the steady-state temperature profiles in the columns for all the design cases. These will be used in the control studies discussed in the following sections.

4. Reflux Ratio and Reflux-to-Feed Structures

When a single temperature is controlled in a distillation column, the two most commonly used control structures are (1) maintaining a constant reflux ratio or (2) maintaining a constant reflux-to-feed ratio. Both of these structures effectively handle feed-rate changes,

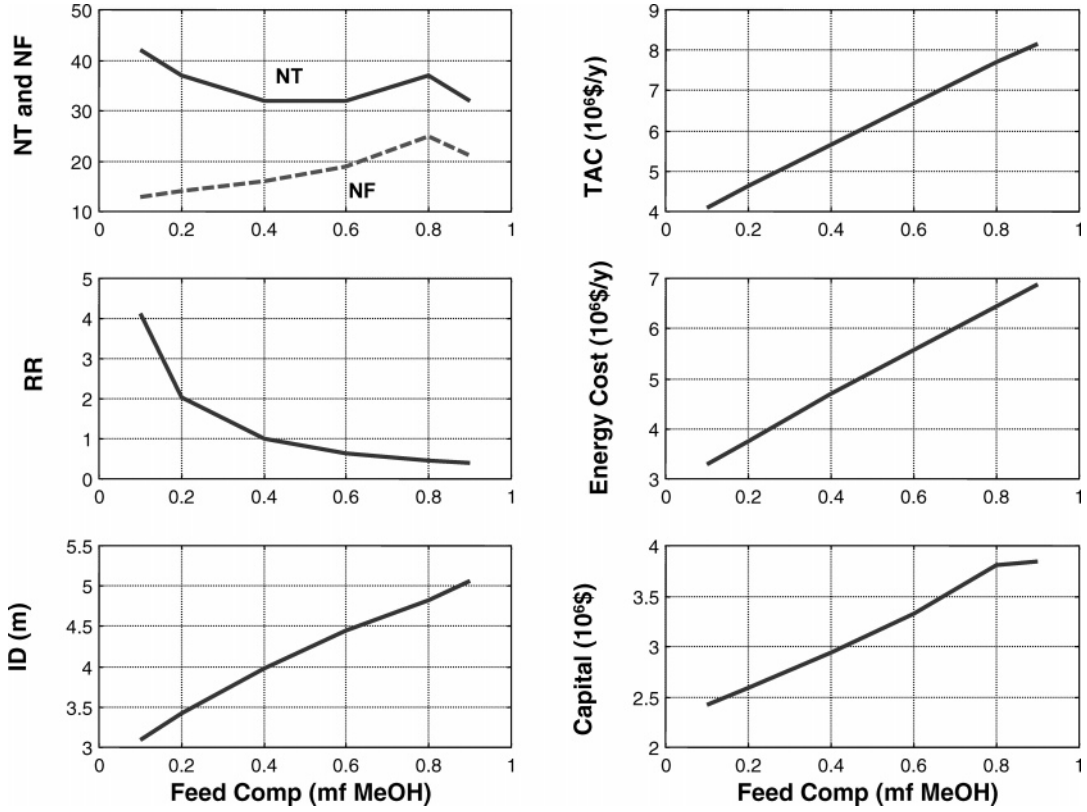

Figure 1. Optimum steady-state designs.

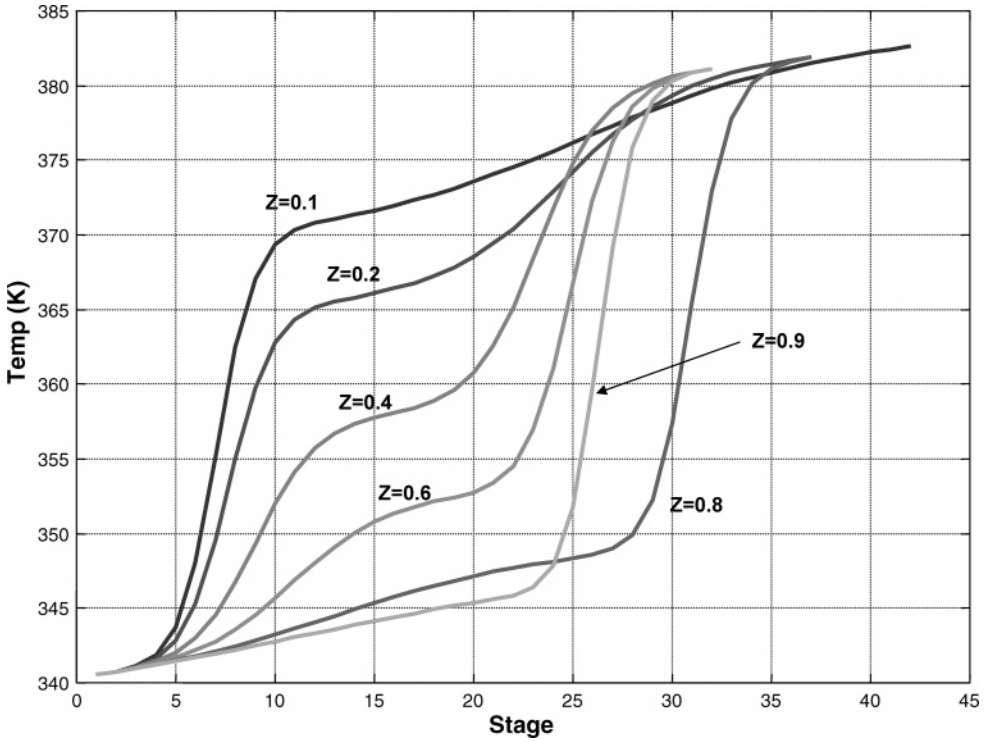

Figure 2. Temperature profiles.

because all flows are scaled up and down with the feed flow rate. However, their effectiveness in handling feed compositions is usually quite different. There are systems in which the constant reflux ratio provides better product-purity control for changes in feed composition. However, in my experience, the constant reflux-to-feed structure provides superior performance in a majority of systems.

The difference between the two structures can be quantitatively evaluated by using a steady-state simulation.[1] The procedure is as follows:

1. Start with the design feed composition.

2. Fix the purities of both the distillate and the bottoms by adjusting the distillate-to-feed ratio and the reflux ratio. In Aspen Plus, this is done by using the "Design-Spec/Vary" feature.

Table 3. Comparison of Reflux Ratio and Reflux-to-Feed Structures (for Feed Flow Rate = 1 kmol/s)

design feed comp. z (mf MeOH)	z	reflux-to-feed ratio	reflux ratio
0.1	0.05	0.4095	8.341
	0.08	0.4094	5.172
	0.10	0.4076	4.109
	0.12	0.4061	3.406
	0.15	0.4049	2.712
0.4	0.35	0.4068	1.163
	0.4	0.4013	1.004
	0.45	0.3981	0.8846
0.9	0.85	0.3676	0.4321
	0.9	0.3567	0.3960
	0.95	0.3303	0.3474

3. Run a number of steady-state cases with different feed compositions.

4. Plot the resulting reflux flow rates and reflux ratios that are required to maintain product purities over this range of feed compositions.

5. Select the variable with the lesser variability.

The results of applying this method to the methanol/water system are given in Table 3 for design cases with three different feed compositions. For the 10 mol % methanol feed design case, the feed composition is varied from 5 to 15 mol %, and the required reflux ratio and reflux-to-feed ratio are calculated. The changes in the reflux-to-feed ratio are much smaller than those of the reflux ratio. The reflux-to-feed ratio only changes ~1% over the entire range of feed compositions, while the reflux ratio changes by a factor of 3.

These results indicate that the constant reflux-to-feed strategy will maintain product purities closer to their specified values. Similar results for other design feed cases (40 and 90 mol % methanol) are also shown in Table 3. The higher the feed composition, the smaller the difference between the two structures. For example, in the 90 mol % case, the change in the reflux ratio is ~34% while the change in the reflux-to-feed is ~11%.

It is clear that the reflux-to-feed structure is preferred in the methanol/water separation, particularly at low feed compositions. The dilemma is that, at the low feed compositions, the reflux ratio is high. Conventional wisdom says that, in high reflux ratio columns, the reflux-drum level should be controlled by reflux. This precludes the use of a reflux-to-feed structure. So there is a conflict between these two suggested control structures. In the next section, we propose a control structure that satisfies both objectives.

Since the small feed composition case presents the most serious conflict between the RR and *R*/*F* structures, we begin with an examination of this case. The control of a single tray temperature with the two ways to manage the reflux will be tested. In subsequent sections, other feed compositions will be explored, and we will find that the most effective control structure changes as the feed composition changes.

5. Feed Composition 10 mol % Methanol

The economic optimum column has 42 total stages and is fed on Stage 13. The important parameter in this case is the reflux ratio, which is high at 4.11 because the distillate flow rate is small (only 10% of the feed).

The first issue is the selection of which tray temperature to control. A common distillation control heuristic is to select a tray where the change in temperature from tray to tray is the largest (steep temperature profile). Figure 2 gives temperature profiles for all the cases. The $z = 0.1$ profile has its maximum slope at Stage 7. Note that this is above the feed stage in the rectifying section. At this location, either the reflux or the vapor boilup can be used to control temperature. Changes in vapor rates affect the temperatures on all trays quickly, so vapor boilup can be used to control a temperature at any location in the column. Changes in reflux have significant hydraulic lags (3−6 s per tray), so using reflux to control a temperature far down in the column should be avoided. However, in this case, Stage 7 is only six trays down in the column, so reflux could be used.

5.1. S7-RR Structure. We start by assuming that the high reflux ratio requires the control of the reflux-drum level by manipulating the reflux flow rate. Figure 3A gives the Aspen Dynamics flowsheet and shows the controller faceplates. The distillate flow rate is ratioed to the reflux flow rate (note in the "FCD" faceplate that this controller is on "cascade"). Stage 7 is controlled by manipulating the reboiler heat input. A 1-min deadtime is used in the temperature loop, and 100-K temperature transmitter spans are used. The relay-feedback test is run to determine the ultimate gain and period, and the Tyreus−Luyben tuning rules are used ($K_C = 0.67$ and $\tau_I = 13$ min). The column base and the reflux drum are sized to give 5-min holdup times when 50% full, based on the total liquid entering or leaving. Proportional level controllers with $K_C = 2$ are used.

This RR control structure handles changes in feed flow rate quite well. However, it does not handle disturbances in feed composition. Figure 4 gives product-purity results for several control structures. The curves labeled "S7−RR" refer to the structure in which the reflux ratio and the Stage 7 temperature are controlled. An increase in the feed composition from 10 to 12 mol % methanol (the left two graphs) does not cause a problem in terms of the purities of both the bottoms and distillate purities. Both the distillate purity x_D and the bottoms purity x_B remain near the desired 0.999 mf. However, a decrease in the feed composition from 10 to 8 mol % methanol (the right two graphs) produces a drastic drop in the purity of the bottoms. Clearly, this structure does not provide effective control of product purities for feed-composition disturbances.

5.2. S25-RR Structure. Since a temperature near the top of the column is being controlled, it is reasonable that the distillate purity stays fairly close to its specification, while the bottoms purity does not. One might conclude that a tray down further in the column might give better control of the bottoms purity. Looking again at the temperature profile for the $z = 0.1$ case in Figure 2, we can see another region where the temperature is changing from tray to tray. This occurs at Stage 25, which is much lower in the column. The temperature controller is retuned, giving $K_C = 4.3$ and $\tau_I = 5.3$ min. Note that this gain is larger than the previous gain when Stage 7 temperature is controlled, which is due to the smaller process gain on Stage 25 (temperature profile less steep).

Results for using this control tray are also shown in Figure 4 in the curves labeled "S25−RR." This structure does a good job in controlling the bottoms composition for both positive and negative changes in the feed composition. However, now the distillate purity drops drastically for an increase in feed composition.

We could conclude that, if the distillate purity is more important than the bottoms purity, the S7−RR struc-

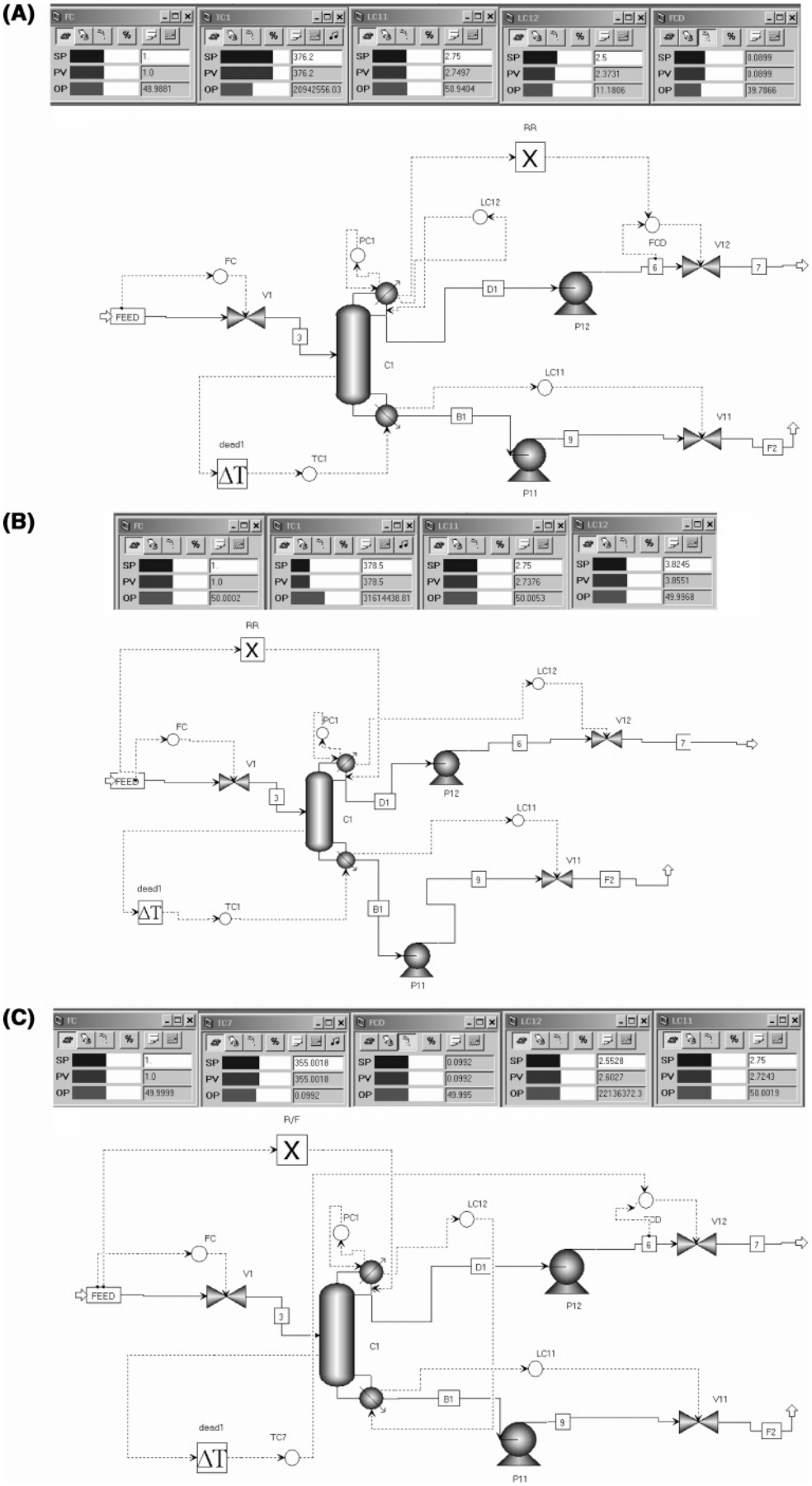

Figure 3. (A) RR control structure with temperature control using Q_R. (B) R/F control structure with temperature control using Q_R. (C) R/F control structure with temperature control using D.

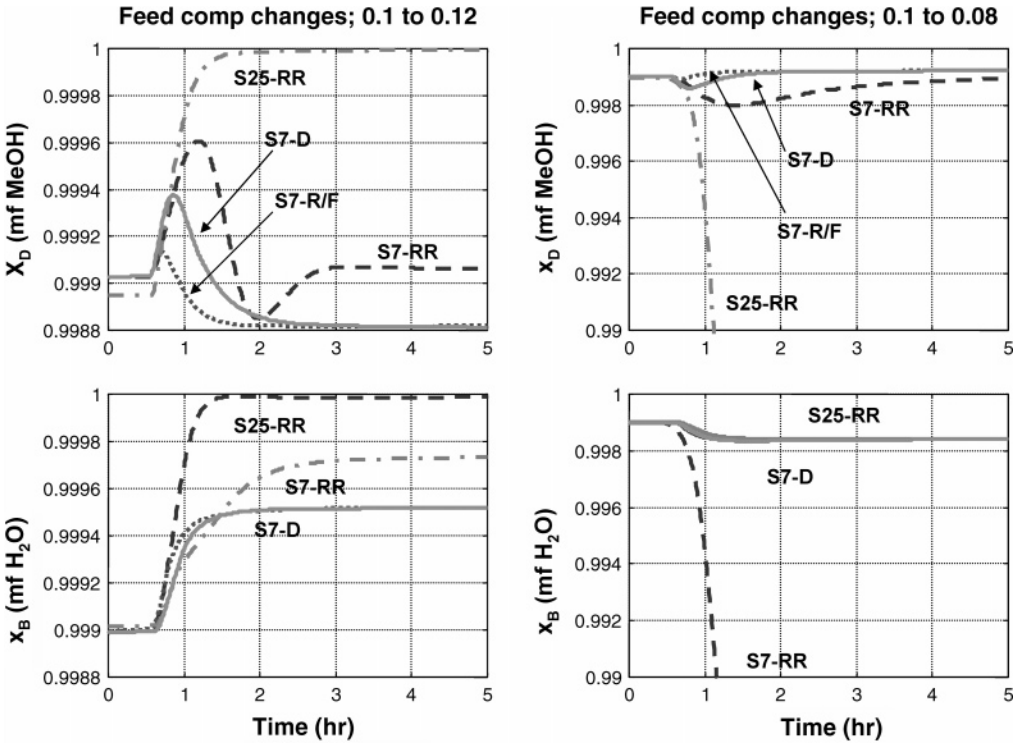

Figure 4. Feed-composition changes ($z = 0.1$).

ture should be used. On the other hand, if the bottoms purity is more important than the distillate purity, the S25−RR structure should be used. But what do we do if both purities are important? This is usually the case in most industrial methanol/water separations. The methanol is a product or a recycle stream that typically must be quite pure. The bottoms stream is often a waste product in which only very small amounts of methanol can be tolerated because of yield losses and pollution regulations. The basic problem is that the steady-state calculations given in Section 4 have revealed that the reflux ratio has to change for changes in feed composition.

5.3. S7-*R/F* Structure. Since the RR schemes do not work well, let us evaluate the reflux-to-feed *R/F* scheme, despite the fact that we have a high reflux ratio. Figure 3B shows the control structure. The reflux-drum level is controlled by manipulating the small distillate flow rate. Stage 7 temperature is controlled by manipulating the reboiler heat input. The flow rate of the reflux is ratioed to the feed flow rate (using a mass ratio, since Aspen Dynamics permits setting the mass flow rate of the reflux).

The curves labeled "S7-*R/F*" in Figure 4 show that this inherently superior *R/F* structure can handle feed-composition disturbances very well. However, remember that the distillate flow rate is only 0.1 kmol/s, while the reflux flow rate is 0.4 kmol/s. Suppose a disturbance in vapor boilup requires a 10% change in reflux if the reflux-drum level is controlled by the reflux. The same disturbance would produce a 40% change in distillate if the reflux-drum level is controlled by the distillate. Thus, the variability in the distillate flow rate is potentially quite large. If the distillate is feeding a downstream unit, large changes in the distillate flow rate will subject this downstream process to large load disturbances.

So is it possible to retain the inherently superior reflux-to-feed structure and at the same time avoid controlling the reflux-drum level with the distillate? The control structure proposed in the next section achieved these objectives.

5.4. S7-*D* Structure. Figure 3C shows a control scheme in which the reflux-to-feed ratio, the Stage 7 temperature, and the reflux-drum level are controlled. Instead of using the reflux or the distillate to control the reflux-drum level, the reboiler heat input is chosen as the manipulated variable. Vapor boilup has an immediate and strong effect on the reflux-drum level, so it can provide effective control.

Since reboiler heat input is no longer available to control temperature, the distillate flow rate is selected. Of course, the temperature controller must be retuned for this new configuration. We must remember that the tuning of the temperature controller is affected by the tuning of the reflux-drum level controller in this structure. Column temperatures are *directly* affected by vapor boilup and reflux flow rate. They are only *indirectly* affected by distillate flow rate through its effect on the reflux-drum level, which changes the reflux flow rate if the level controller is on automatic. The level loop is "nested" inside the temperature loop, so the temperature controller cannot work unless the level controller is on automatic. A slow-acting level controller will produce a slow-acting temperature loop.

Therefore, the gain of the proportional level controller is set at 4 to give tighter level control. The resulting tuning of the Stage 7 temperature controller manipulating distillate flow rate is $K_C = 2$ and $\tau_I = 28$ min. Note that this reset time is much larger than when the reboiler heat input is the manipulated variable.

The solid curves in Figure 4 labeled "S7-*D*" give results for this control structure. It gives excellent performance for both composition disturbances.

Figure 5 shows the responses of several important variables when the S7-*R/F* control structure is used. The feed-composition disturbances in Figure 5 are from 10 mol % methanol up to 12 mol % or down to 8 mol %.

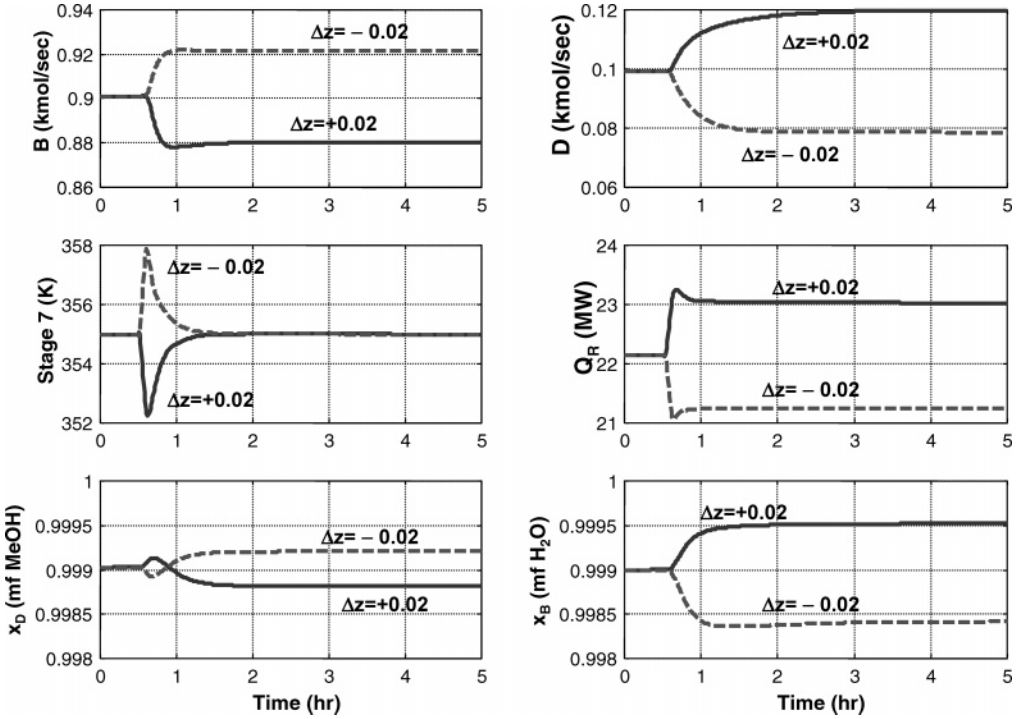

Figure 5. S7-*R*/*F*: feed-composition changes ($z = 0.1$).

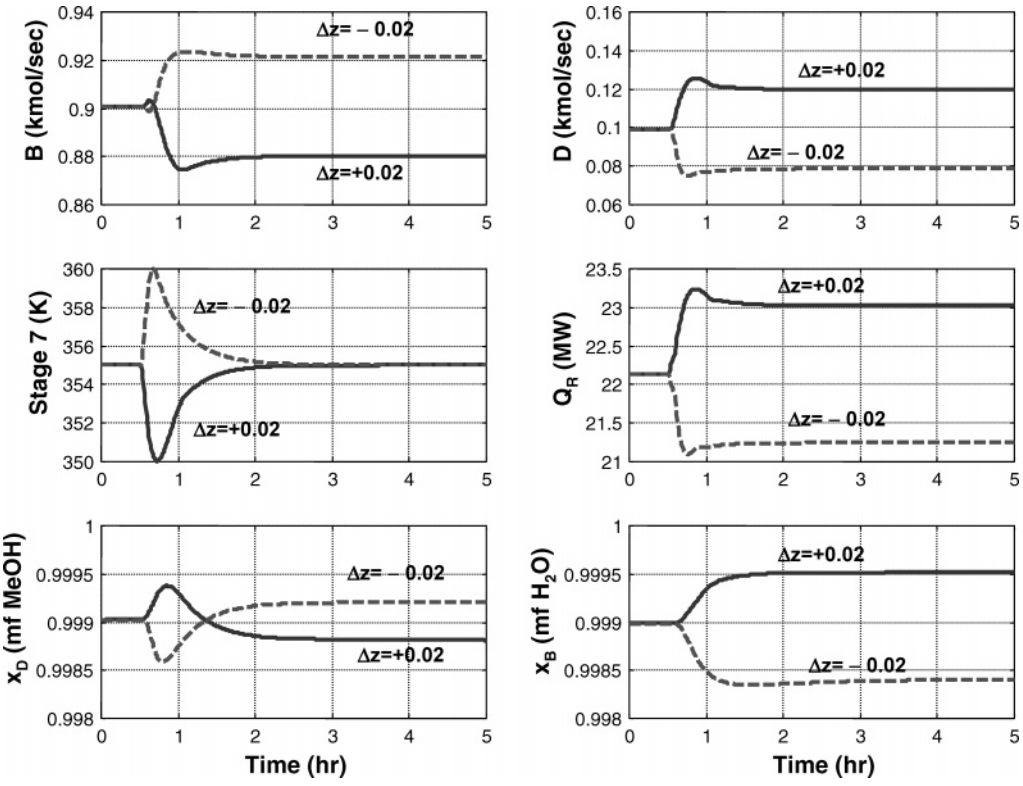

Figure 6. S7 controlled by *D*: feed-composition changes ($z = 0.1$).

Note the smooth changes in the flow rates of both of the product streams because of the proportional level controllers.

Figure 6 shows the responses of several important variables when the S7-*D* control structure is used for feed-composition disturbances. The magnitudes of the transient deviations in Stage 7 temperature are larger than those for the S7-Q_R structure, but the deviations in the purities of the products are about the same.

Now that we have developed an effective control structure for the case with a 10 mol % methanol feed composition, let us see if this structure is required and is effective for higher feed compositions.

6. Feed Composition 20 mol % Methanol

The economic optimum column has 37 total stages and is fed on Stage 14. The reflux ratio is 2.044, which is small enough so that the reflux-drum level can be controlled by either the distillate or the reflux. The temperature profile for the $z = 0.2$ case, given in Figure 2, shows a steep profile at Stage 7 in the rectifying

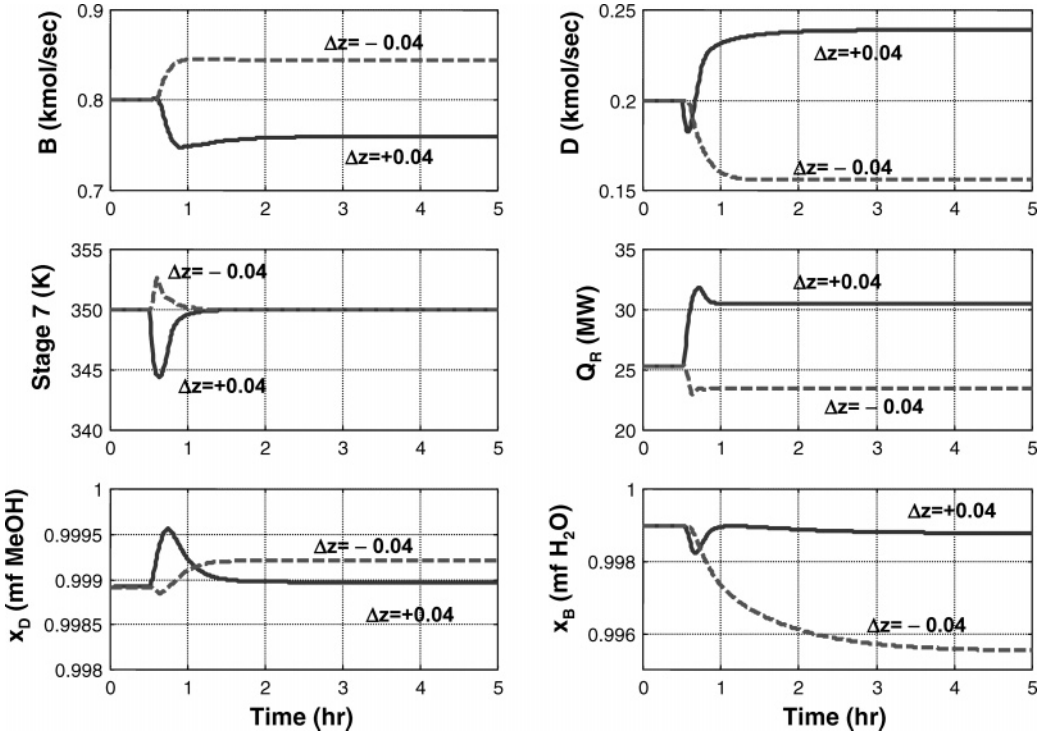

Figure 7. S7 *R*/*F*: feed-composition changes ($z = 0.2$).

section. Therefore, we use the reflux-to-feed ratio and control Stage 7 with the vapor boilup.

The effectiveness of this structure is illustrated in Figure 7 for composition disturbances. The feed composition is changed from 20 mol % methanol to 24 mol % or 16 mol %. The increase in feed composition is well-handled. The decrease causes the bottoms purity to drop from 99.9 mol % methanol to a little below 99.6 mol % methanol, which is still reasonably close to specification.

These results indicate that controlling a suitable tray temperature and using a reflux-to-feed ratio provides quite effective control for the 20 mol % feed-composition system.

Now let us see what happens as we go to still higher feed compositions.

7. Feed Composition 40 mol % Methanol

The economic optimum column has 32 total stages and is fed on Stage 16. The reflux ratio is 1.044, so the reflux-drum level can be controlled by either the distillate or the reflux. The temperature profile for the $z = 0.4$ case given in Figure 2 shows that the location of the steepest part has shifted to the stripping section of the column (Stage 24).

7.1. S24-R/F Structure. We start by evaluating the control structure that uses a reflux-to-feed ratio and controls Stage 24 with the vapor boilup. This is a single-end control structure in which one temperature is controlled and the other degree of freedom is used to set the reflux flow rate. The temperature controller tuning constants are $K_C = 3.8$ and $\tau_I = 6.6$ min.

Figure 8 gives results for feed-composition disturbances from 40 mol % methanol up to 48 mol % and down to 32 mol %. The solid curves labeled "S24" are for the case when Stage 24 is controlled. The increase in feed composition can be handled, but the decrease results in the distillate purity dropping below 98 mol %. Remember that the temperature being controlled is now in the stripping section, so the control of the bottoms purity should be better than that of the distillate purity.

Suppose we select a tray in the rectifying section where there is a reasonably steep temperature profile. The responses shown in the dashed curves in Figure 8 labeled "S9" are achieved by using Stage 9 and retuning the temperature controller ($K_C = 4.7$ and $\tau_I = 7.9$ min). Now the bottoms purity drops below 98 mol % for the feed-composition decrease.

These results show that, despite using the preferred reflux-to-feed structure, a single-temperature control structure cannot maintain the purities of both products for feed-composition disturbances. Therefore, for columns with a feed composition of 40 mol % methanol, a "dual-temperature" control structure is required.

7.2. Dual-Temperature Structure. The need to control two temperatures creates a more difficult control problem because of the potential for interaction between the control loops. The tuning of two controllers in a 2×2 multivariable system and the selection of what two temperatures to control require more analysis than a simple single-temperature SISO (single-input, single-output) structure. Certainly, simplicity is a very desirable feature in any process control system. However, the requirements of the process dictate that a more complex control structure is needed for the methanol/water separation when the feed composition is around 40 mol % methanol.

7.2.A. Selection of Control Tray Locations. The first issue is to select two appropriate tray locations for temperature control. Singular value decomposition[2] (SVD) gives some guidance for selecting the most sensitive tray locations in a multivariable control structure. The first job is to find the steady-state gain matrix relating all the tray temperatures to the two manipulated variables (reflux and reboiler heat input). These gains can be found numerically using the steady-state simulator. Two runs are required, one for each of the

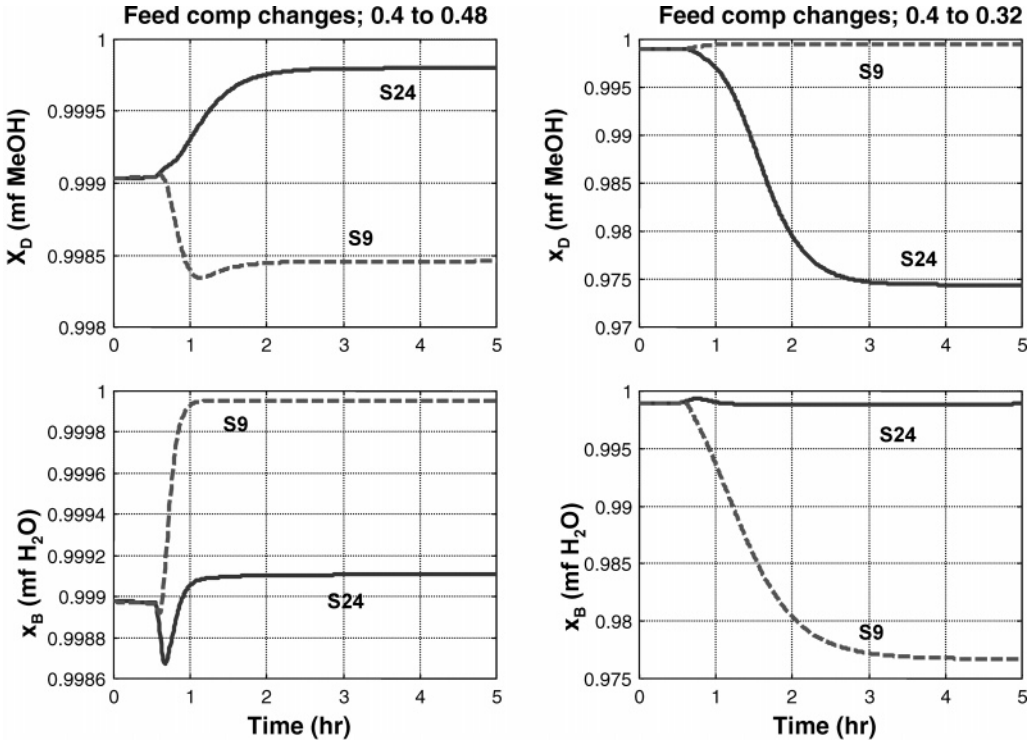

Figure 8. S24 and S9 *R*/*F*: feed-composition changes ($z = 0.4$).

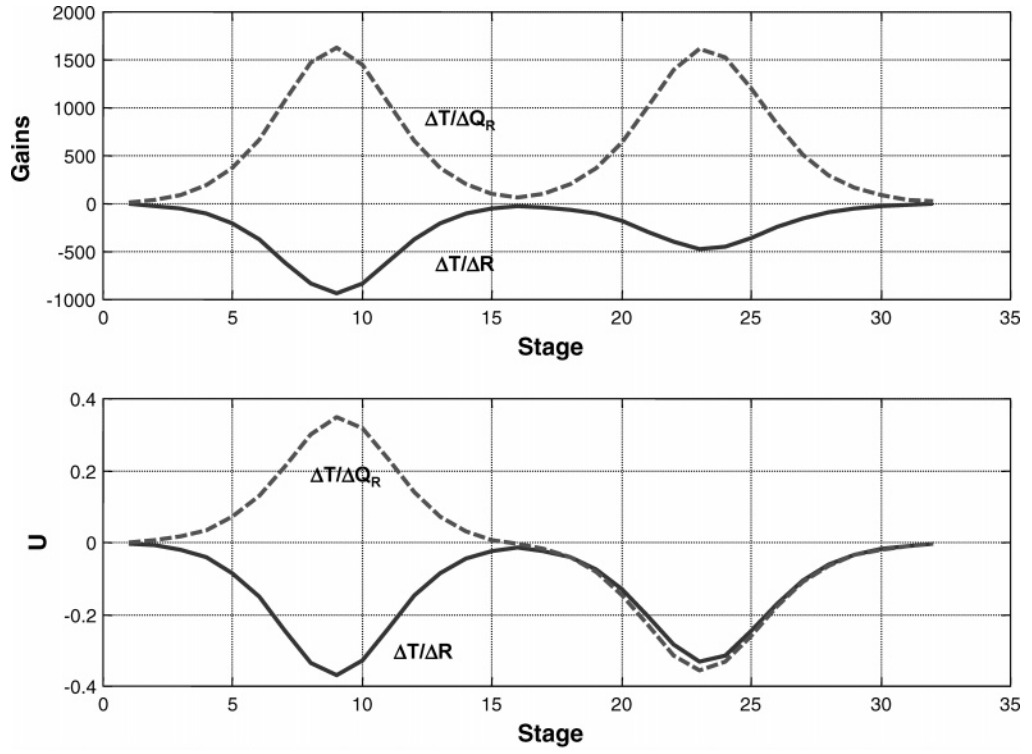

Figure 9. Gains and SVD analysis; 0.01% changes in R and Q_R ($z = 0.4$).

inputs. A very small change (0.01% of the steady-state value) is made in the reflux flow rate with the reboiler heat input fixed. Note that the "Design Spec/Vary" feature is not used for these "open loop" runs. The resulting temperature on each tray is subtracted from the original temperature to calculate the deviation. Dividing this by the change in the reflux gives the open-loop process gain between the tray temperature and the reflux. Then the procedure is repeated for a very small change in the reboiler heat input with the reflux flow rate fixed.

These steady-state gains are shown in the upper graph in Figure 9. The dashed curves are for changes in the reboiler heat input Q_R. The solid curves are for changes in the reflux R. As expected, the gains are positive for Q_R and negative for R. The steady-state gain matrix is decomposed, using the SVD function in Matlab. The resulting two vectors of the U matrix are given in the lower graph in Figure 9. The peaks in the U curves indicate the most sensitive stages from a steady-state standpoint. Stages 9 and 24, which we used for the single-temperature control structures based on

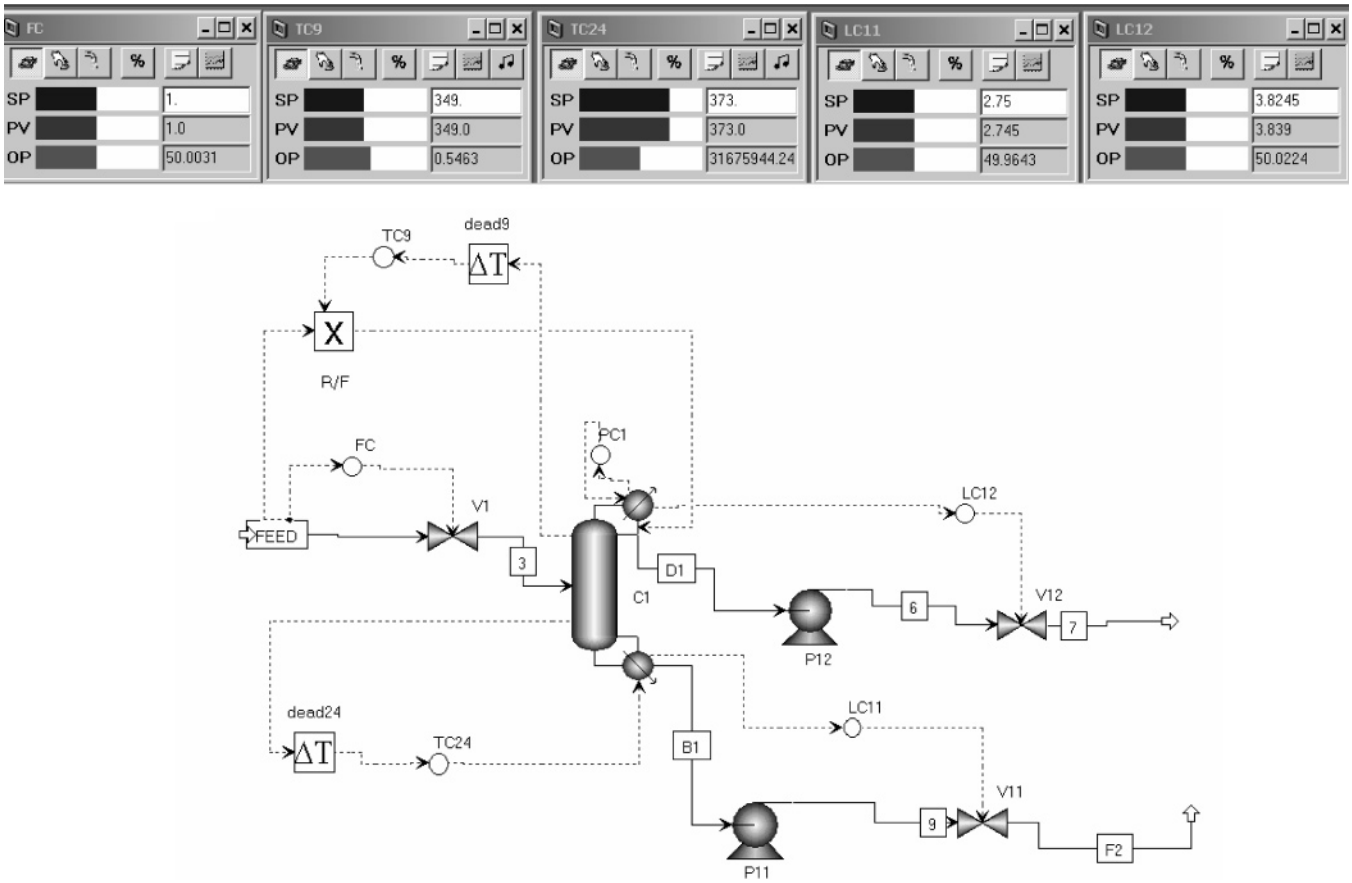

Figure 10. Dual-temperature control, S9-R and S24-Q_R.

simply looking at the shape of the temperature profile, are located at or very near the peaks.

The magnitudes of the R and Q_R peaks in the U curves are not significantly different, so SVD analysis suggests that either set of pairings could be used. However, a common-sense consideration of the dynamics suggests that we select the reflux to control the temperature of Stage 9 near the top of the column and the reboiler heat input to control the temperature of Stage 24 near the bottom. Note that the Stage 9 controller is direct acting, and the Stage 24 controller is reverse acting.

7.2.B. Controller Tuning. The second issue is to tune the controllers in the multivariable environment. A "sequential" method is used in this paper. The reflux flow rate is fixed, and the Stage 24 temperature controller is tuned using a relay-feedback test and the Tyreus–Luyben tuning constants (which are $K_C = 3.8$ and $\tau_I = 6.6$ min, the same as reported previously for SISO control). This loop is selected to tune first because the dynamics between the temperature and the reboiler heat input are faster than the dynamics between the temperature and the reflux.

Then the Stage 24 temperature controller is put in automatic, and the Stage 9 temperature controller is relay-feedback tested. The resulting Tyreus–Luyben controller constants are $K_C = 3.3$ and $\tau_I = 19$ min. Note that this tuning is significantly different that that obtained for the SISO system with Stage 24 controlled by the reboiler heat input ($K_C = 4.7$ and $\tau_I = 7.9$ min). This illustrates the impact of controller interaction and manipulated variable selection. Figure 10 gives the dual-temperature control scheme. The T24 controller manipulates the reboiler heat input. The T9 controller manipulates the reflux-to-feed ratio.

The effectiveness of this control structure for feed-composition disturbances is compared with the single-temperature results in Figure 11. The solid curves are the dual-temperature case. Both product purities are maintained quite close to the desired 99.9 mol % specification for both positive and negative feed-composition changes. More details of the dual-temperature control response are given in Figure 12 for feed-composition changes. Both Stage 9 and Stage 24 temperatures are well-controlled with maximum deviations of only ~2 K. The increases and decreases in the flow rates of the product streams leaving the column are gradual and without overshoot, so downstream units are not subjected to severe disturbances.

Now let us see what kind of control structure is needed for a column that is designed for a feed composition of 60 mol % methanol.

8. Feed Composition 60 mol % Methanol

The economic optimum column has 32 total stages and is fed on Stage 19. The reflux ratio is 0.604, so we control the reflux-drum level by manipulating the distillate. The temperature profile for the $z = 0.6$ case given in Figure 2 shows a steep profile at Stage 26 in the stripping section.

Therefore, if a single temperature control structure is used, the reflux-to-feed ratio is maintained and the temperature on Stage 26 is controlled by manipulating the reboiler heat input. Controller tuning gives $K_C = 1.6$ and $\tau_I = 7.9$ min).

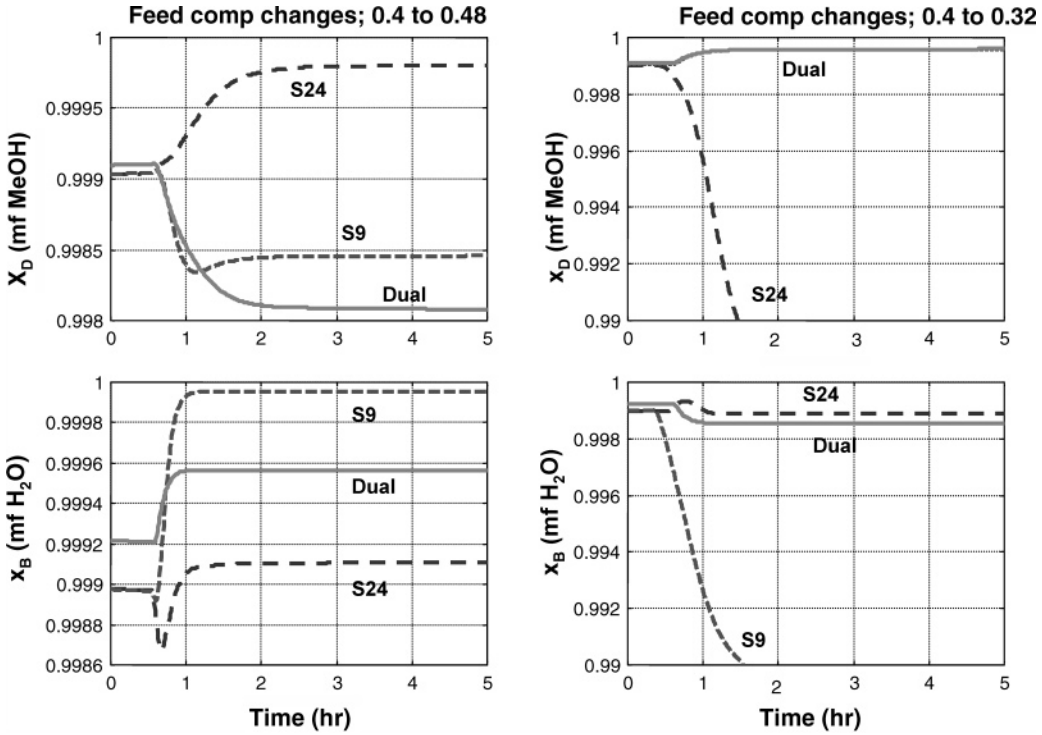

Figure 11. S24, S9 and dual-temperature control: feed-composition changes ($z = 0.4$).

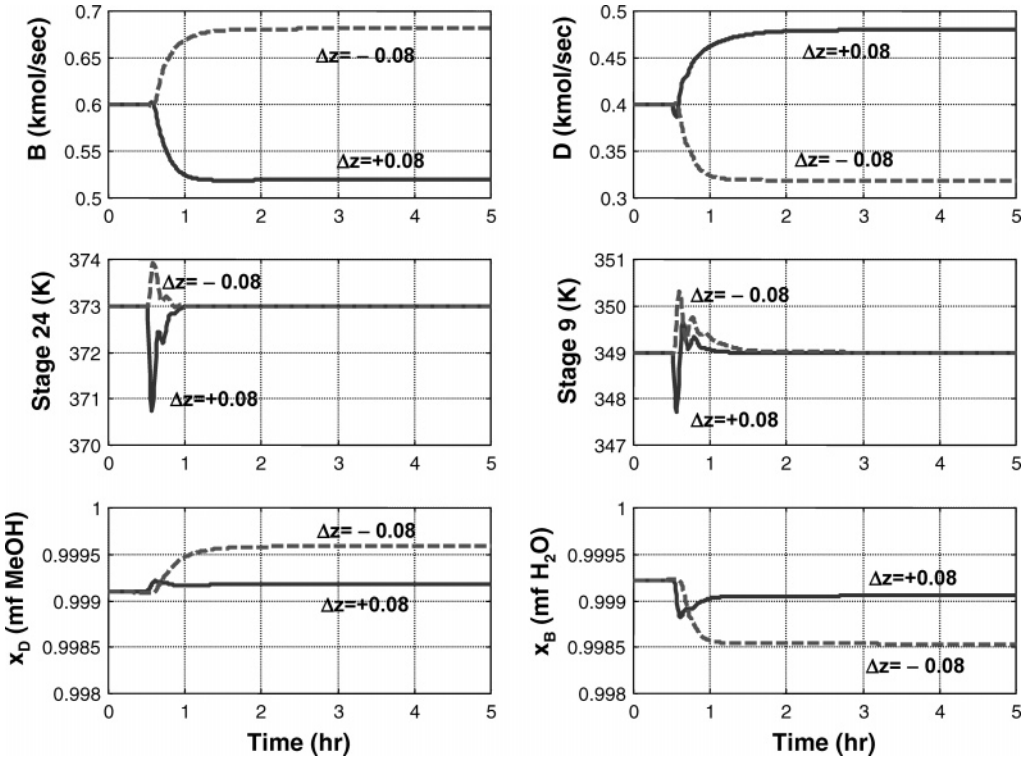

Figure 12. Dual-temperature control, *R*/*F*: feed-composition changes ($z = 0.4$).

The effectiveness of this SISO structure is given in Figure 13 (the dashed lines) for feed-composition changes from 60 mol % to 68 mol % and from 60 mol % to 52 mol % methanol. The purity of the distillate drops below 99 mol % for the decrease in feed composition. So dual-temperature control is needed.

Stage 11 is selected for the second control tray and is controlled by manipulating the reflux-to-feed ratio. Sequential tuning gives controller settings for this loop of $K_C = 4.5$ and $\tau_I = 21$ min.

The effectiveness of this 2 × 2 structure (the solid lines) is compared with the SISO structure in Figure 13 for feed-composition changes. The dual-temperature control structure does an excellent job in maintaining product purities. More details are given in Figure 14, which shows the responses to feed-composition disturbances.

Let us now see what happens for even larger feed compositions.

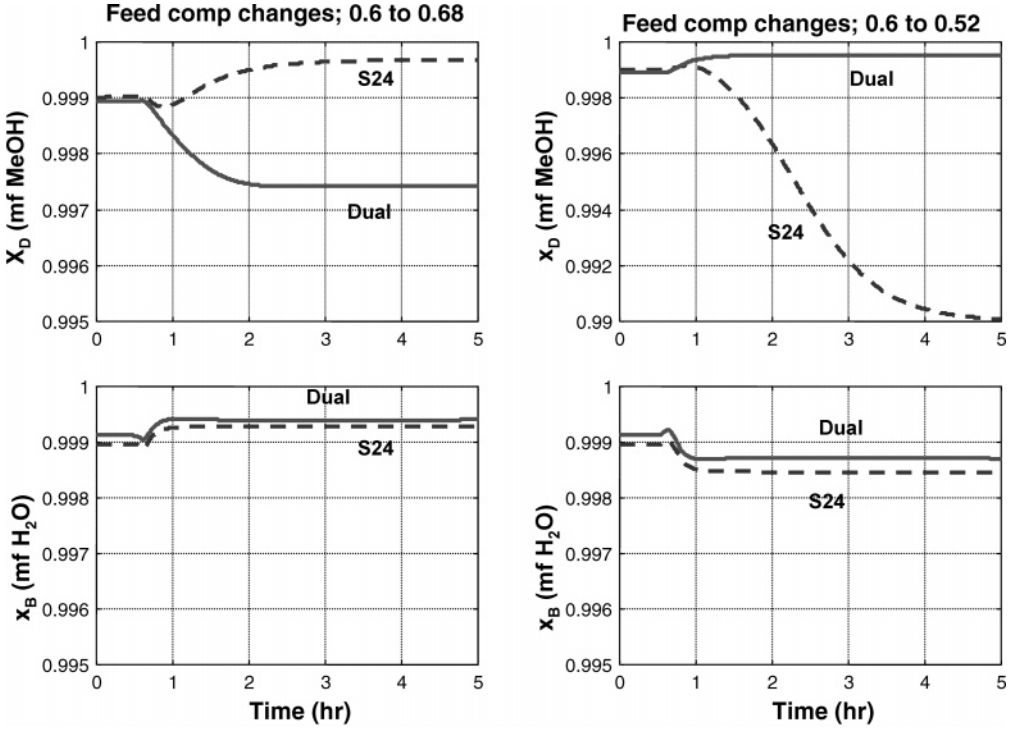

Figure 13. S29 and dual-temperature control, *R*/*F*: feed-composition changes ($z = 0.6$).

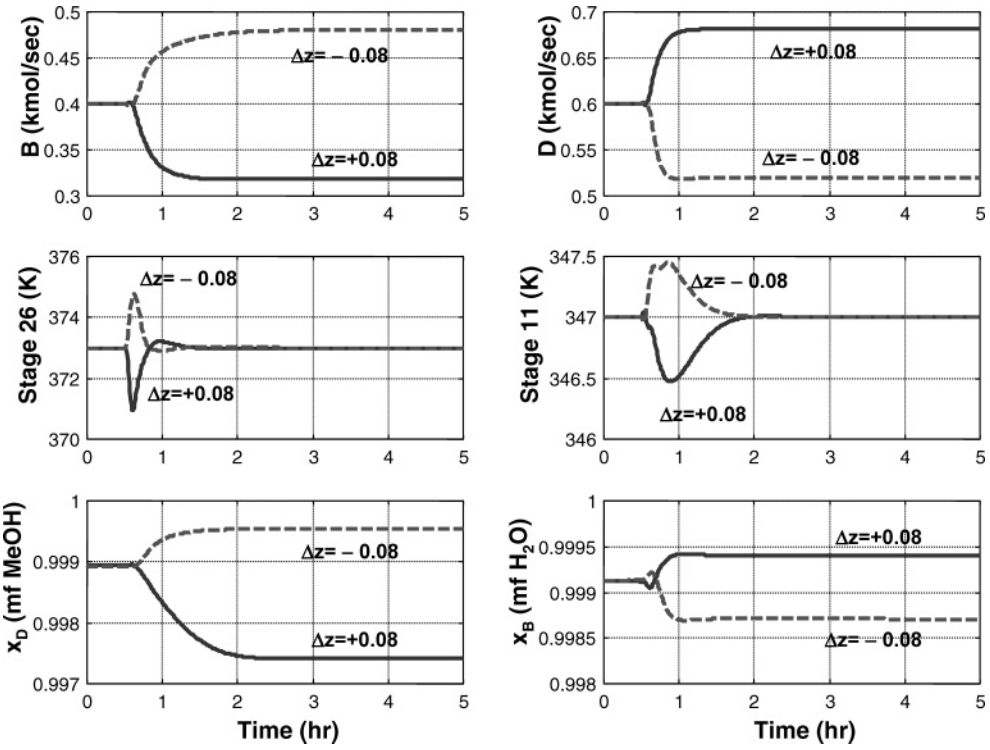

Figure 14. Dual-temperature control, *R*/*F*: feed-composition changes ($z = 0.6$).

9. Feed Composition 80 and 90 mol % Methanol

9.1.A. 80 mol % Feed. The economic optimum column for an 80 mol % methanol feed has 37 total stages and is fed on Stage 25. The reflux ratio is 0.456, so we control the reflux-drum level by manipulating the distillate. The temperature profile for the $z = 0.8$ case given in Figure 2 shows a steep profile at Stage 31 in the stripping section. Note that this is quite close to the bottom of the column.

Therefore, if a single-temperature control structure is used, the reflux-to-feed ratio is maintained and the temperature on Stage 31 is controlled by manipulating the reboiler heat input. Controller tuning gives $K_C = 1.3$ and $\tau_I = 9.2$ min.

The effectiveness of this SISO structure is given in Figure 15 for feed-composition changes from 80 mol % to 84 mol % and from 80 mol % to 76 mol % methanol. These disturbances are handled well. The decrease in

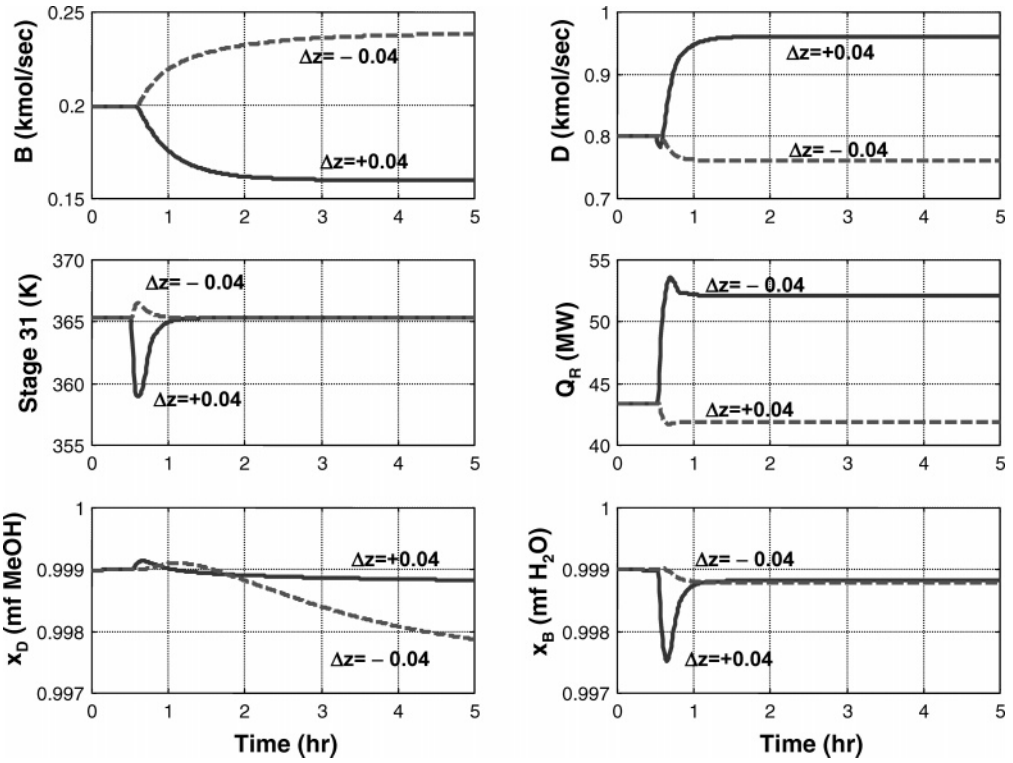

Figure 15. S31 *R*/*F*: feed-composition changes ($z = 0.8$).

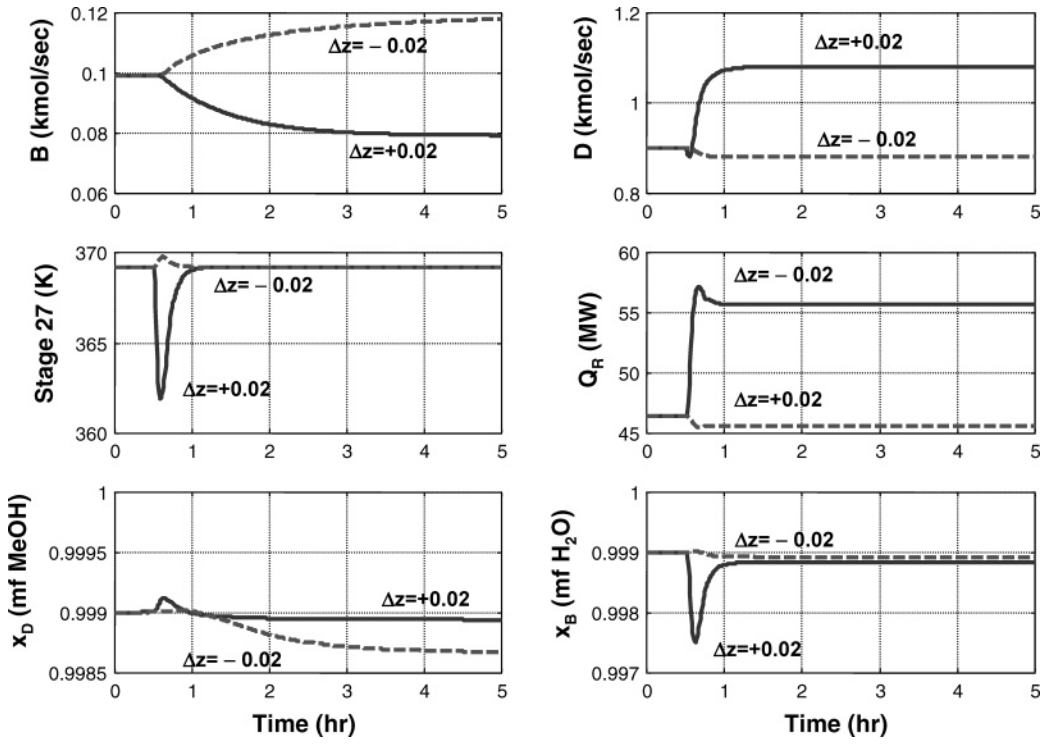

Figure 16. S27 *R*/*F*: feed-composition changes ($z = 0.9$).

feed composition results in a slow decrease in the distillate purity, but it only drops to ~99.75 mol % methanol.

9.1.B. 90 mol % Feed. The economic optimum column for a 90 mol % methanol feed has 32 total stages and is fed on Stage 21. The reflux ratio is 0.396, so we control the reflux-drum level by manipulating the distillate. The temperature profile for the $z = 0.9$ case given in Figure 2 shows a steep profile at Stage 27 in the stripping section.

Therefore, if a single-temperature control structure is used, the reflux-to-feed ratio is maintained and the temperature on Stage 27 is controlled by manipulating the reboiler heat input. Controller tuning gives $K_C = 1.8$ and $\tau_I = 7.9$ min.

The effectiveness of this SISO structure is given in Figure 16 for feed-composition changes from 90 mol % to 92 mol % and from 90 mol % to 88 mol % methanol. Both disturbances are handled well.

These results indicate that a dual-temperature control structure is not needed at high feed concentrations.

10. Other Systems

The numerical example used in this study is the methanol/water separation, which has nonideal vapor−liquid equilibrium and relative volatilities that range from ~2 to 5 over the composition space. We also consider high-purity products (99.9%). Are the results applicable to other systems?

We believe the results can be extended to other chemical systems that produce high-purity products. Several other systems have been studied, and results indicate that there is less need for dual-temperature control in columns producing low-purity products.

For example, a propane/isobutane separation was studied with product purities of 98%. The economic optimum column for a feed composition of 40 mol % propane has 37 stages and operates at 13.5 atm with a reflux ratio of 2.73. The constant reflux-to-feed ratio is preferred in this system. Controlling a single tray temperature (Stage 7) and changing feed composition over the range of 32−48 mol % propane resulted in changes in distillate purity from 98.41 to 97.51 mol % propane and changes in bottoms purity from 98.08 to 98.77 mol % isobutane. If these fairly small changes in product purities are acceptable, there is no need for dual-temperature control. Similar results were seen in the benzene/toluene system. The results of this paper are limited to high-purity columns.

11. Conclusion

This paper presents a methodology for exploring the effect of feed composition on control structure for a binary, high-purity distillation column that depends on the feed composition. The binary distillation of methanol/water is used as a numerical example in this paper, but the results should be applicable to many binary separations.

Dual-temperature control is required for intermediate feed compositions, but single-temperature control is adequate for either low or high feed compositions. For the methanol/water separation, the reflux-to-feed structure should be used throughout the range of feed compositions. At low feed compositions, this presents a dilemma because of the high reflux ratio, which normally requires that the reflux be used to control the reflux-drum level. A control structure is proposed that overcomes this difficulty: control the reflux-drum level with the reboiler heat input and control a tray temperature with the distillate. Fortunately, the location of the appropriate control tray is up in the rectifying section, so temperature control using the distillate is effective.

Dynamic simulations have been used to assess control structure effectiveness. It should be noted that, if one is only interested in the steady-state effect of changing feed composition with a given control structure, a steady-state simulation can be used. For example, if the fixed reflux-to-feed and single-tray-temperature control structure is to be evaluated, the "Design Spec-Vary" capability in Aspen Plus can be used with the reflux flow rate fixed and the selected stage temperature fixed. Then feed composition is changed over the expected range, and the new steady-state values of x_D and x_B show how much change there is in product purities as the feed composition changes.

Nomenclature

AC = heat transfer area of condenser (m^2)
AR = heat transfer area of reboiler (m^2)
B = bottoms flow rate (kmol/sec)
D = distillate flow rate (kmol/sec)
HX = heat exchanger
ID = column diameter (m)
L = length of column (m)
NF = feed stage
NT = total number of stages
QC = condenser heat removal (MW)
QR = reboiler heat input (MW)
R = reflux flow rate (kmol/sec)
R/F = reflux-to-feed ratio
RR = reflux ratio = R/D
Sn = stage number for temperature control
TAC = total annual cost (10^6 \$/y)
x_B = composition of bottoms product (mf water)
x_D = composition of distillate product (mf methanol)
z = composition of feed (mf methanol)
ΔF = change in feed flow rate
Δz = change in feed composition

Literature Cited

(1) Luyben, W. L. Steady-state energy-conservation aspects of distillation control system design. *Ind. Eng. Chem. Fundam*. **1975**, *14*, 321.

(2) Moore, C. F. Selection of controlled and manipulated variables. In *Practical Distillation Control*; Van Nostrand Reinhold: New York, 1992; Chapter 8.

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