

PROCESS DESIGN AND CONTROL

Guides for the Selection of Control Structures for Ternary Distillation Columns

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This paper presents a methodology for the selection of effective control structures for ternary distillation columns using only temperature measurements. A fundamental choice between controlling a single temperature or two temperatures must be made. If the former is selected, an additional choice between reflux-ratio control and reflux-to-feed control must also be made. The procedure discussed in this paper uses steady-state rating calculations to guide these selections. With product purities fixed (the impurity of the heavy key component in the distillate and the impurity of the light key in the bottoms), a steady-state simulator is used to calculate the required changes in the reflux flowrate and the reflux ratio as feed composition is varied over an anticipated range. For a ternary system, two “constant-purity” surfaces in two three-dimensional spaces are generated: (z_A, z_B, RR) and $(z_A, z_B, R/F)$. The structure that has the flatter of the two surfaces should be selected if a single temperature control structure is employed. If neither surface is flat, dual temperature may be required.

1. Introduction

The design of distillation control structures involves a number of choices. If the column is a conventional two-product column, there are two control degrees of freedom remaining after pressure, base level, and reflux-drum level are controlled. This is true for any system (binary, multicomponent, ideal, nonideal, etc.). Theoretically, the compositions of the two product streams should be controlled: the impurity of the heavy key component in the distillate and the impurity of the light key in the bottoms. This would involve two composition analyzers, which are often expensive and raise questions of high maintenance costs and reliability. Therefore, inferential composition control using temperatures is very frequently used.

The first issue is to select the appropriate trays whose temperatures should be controlled. Singular value decomposition methods¹ are useful for this problem. However, do we really need to control two temperatures? The interaction between the two temperature controllers presents more difficult tuning problems. There are no remaining control degrees of freedom. The temperature controllers manipulate two input variables. The most common choices are reboiler heat input and reflux, but other structures are used depending on a number of factors.

In industrial practice, a majority of distillation columns are controlled by using a single temperature somewhere in the column. This more simple structure is quite effective in many systems. However, a degree of freedom remains that must be set. Two common

choices are maintaining a constant *reflux ratio* or maintaining a fixed *reflux-to-feed ratio*. These two alternatives give distinctly different results. It is necessary to select the better of the two.

A method for achieving this in binary distillation was proposed three decades ago² and has been used by control practitioners as a tool to guide in the selection of dual-temperature control versus single-temperature control and in the selection of reflux-ratio control versus reflux-to-feed control.

It is very important to remember that disturbances in feed flowrate can be handled by any of the structures mentioned above. In theory, all flowrates and energy duties scale directly with throughput. This is true if factors such as tray efficiencies, pressure drop, and entrainment do not change with throughput. For example, suppose the feed flowrate increases by 20%. If the reflux flowrate and the reboiler heat input are increased by 20%, the column will come to a new steady state that has the identical compositions and temperatures on all trays. Therefore, if we neglect the possibility of dynamic problems, any control structure that maintains a ratio of flowrates will eventually return the column to the correct steady state. It does not matter if one temperature is controlled or if two temperatures are controlled. Theoretically, no temperature would need to be controlled. However, measurement errors and pressure changes require that the position of the composition or temperature profile must be controlled.

Therefore, the important disturbance in terms of control structure selection is *feed composition*. Changes in feed composition usually produce large changes in product purities if flowrate ratios are maintained. If a tray temperature is controlled, product purities will not be constant. So, an important part of the control

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selection process is determining how the flow ratios should change or how much product purities change when a control structure is specified.

These issues are present in all distillation columns, binary or multicomponent. Let us start with the binary case since it is the easiest to visualize.

It should be noted that there are other important disturbances that impact the performance of distillation columns. These are associated with heat-balance disturbances. Sudden changes in ambient conditions can drop cooling water temperatures, which can upset the column unless an effective pressure control structure is used. Likewise, sudden changes in steam supply pressure can upset the column unless an effective reboiler heat input control structure is used. These issues are discussed in detail by Shinsky.³

The literature in distillation control in recent years is not as extensive as was the case a decade ago. This is due to several factors, not the least of which is the lack of funding for research in distillation, which is considered to be a “mature” technology. Another important factor is the misconception that all the distillation control problems have been solved by the application of model predictive control. The most recent survey of the field was provided in 1997 by Skogestad.⁴ Riggs and co-workers⁵ discuss control configuration selection for several types of columns. Huang and Riggs⁶ compare PI and MPC control of a gas recovery unit. Balasubramhanya and Doyle⁷ explore the use of a traveling wave model for the control of a high-purity column. Chien and co-workers⁸ discuss the control of a two-column heterogeneous azeotropic distillation system. Castellanos-Sahgun and co-workers⁹ study two-point temperature control by combining feedforward, feedback, and internal model control. Most of the recent work has dealt with more complex plantwide systems or more complex control algorithms. The present paper deals with selection of control structures for ternary distillation.

2. Binary Distillation

In a binary separation, a single composition defines any stream. Traditionally the mole fraction of the light component is used. The composition of the feed stream is z , the composition of the distillate is x_D , and the composition of the bottoms is x_B . The operating objective is to maintain the purities of these two product streams.

The following procedure² can provide guidance in the control structure selection problem:

1. Start from the desired steady-state conditions with the design feed composition where there is a *design* reflux flowrate and a *design* reflux ratio.

2. Select a range of expected changes in feed composition z around the design value.

3. Set up the steady-state simulator so that it maintains the compositions of both products. In the commercial process simulator Aspen Plus, this is achieved by using the “Design Spec/Vary” feature.

4. Calculate the reflux flowrate R and the reflux ratio RR for each feed composition. Express the changes in these variables as percentage changes from the design values or normalize them by dividing by the design values.

5. Plot R versus feed composition z and RR versus feed composition z .

6. The curve with the lesser change (flat curve) indicates the inherently superior control structure.

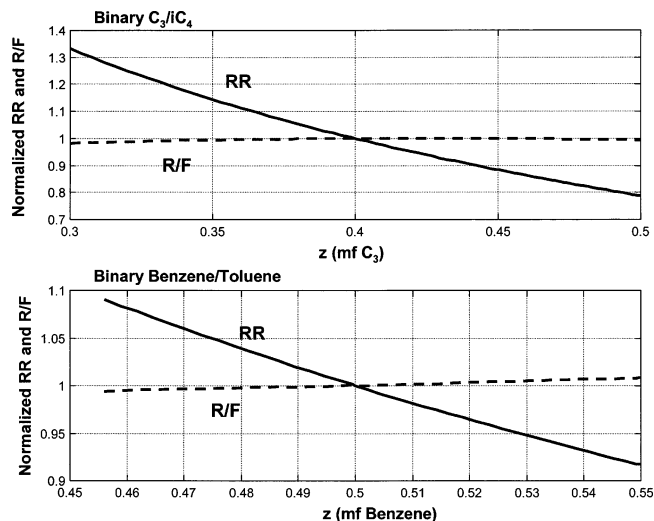


Figure 1. Binary constant-purity curves.

Let us illustrate this procedure with two important examples.

A. Propane–Isobutane Separation. Consider the binary separation of 1 kmol/s of a feed with 40 mol % propane and 60 mol % isobutane in a 37 stage column. We use the Aspen notation of numbering stages from the top of the column with the reflux drum as Stage 1. The feed is introduced on Stage 18. The distillate purity is 98 mol % propane, and the bottoms impurity is 2 mol % propane.

The column operates at 13.5 atm so that cooling water can be used in the condenser. The reflux ratio at design conditions is 2.73, and the reflux-to-feed ratio is 1.08.

The feed composition is varied from 30–50 mol % propane. At each feed composition, the required reflux-to-feed ratio R/F and the reflux ratio $RR = R/D$ are calculated that hold both product streams at their desired compositions.

The reflux-to-feed ratio and the reflux ratio are normalized by dividing by the corresponding design values. Results are given in the top graph in Figure 1. It is clear that the R/F ratio changes very little over the entire feed composition range, while the RR changes about 50%. Thus, control structures with a fixed reflux-to-feed are inherently superior to control structures with a fixed reflux ratio in this system.

B. Benzene–Toluene Separation. Consider the binary separation of 1 kmol/s of a feed with 50 mol % benzene and 50 mol % toluene in a 32 stage column. The feed is introduced on Stage 16. The distillate purity is 99.9 mol % benzene, and the bottoms purity is 99.9 mol % toluene. The column operates at 1 atm. The reflux ratio at design conditions is 1.83, and the reflux-to-feed ratio is 0.917.

The feed composition is varied from 45–55 mol % benzene. At each feed composition, the required reflux-to-feed ratio R/F and the reflux ratio $RR = R/D$ are calculated that hold both product streams at their desired compositions.

Normalized results are given in the bottom graph in Figure 1. It is clear that the R/F ratio changes very little over the entire feed composition range, while the RR changes about 15%. Thus, control structures with a fixed reflux-to-feed are inherently superior to control structures with a fixed reflux ratio in this system.

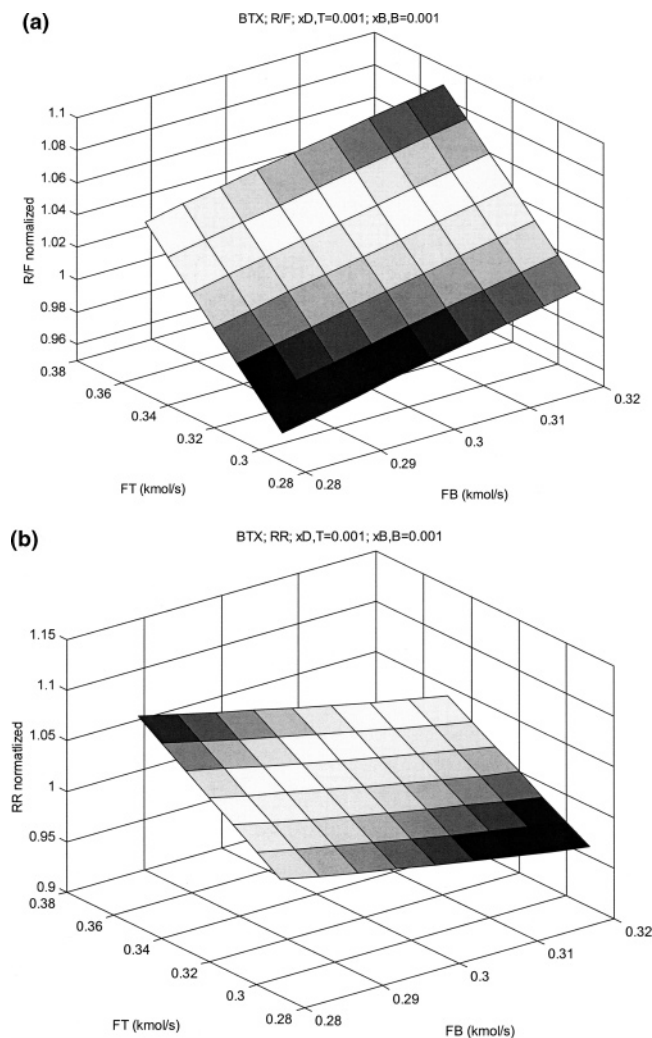


Figure 2. (A) Constant-purity surface: R/F required. (B) Constant-purity surface: RR required.

3. Ternary Systems

The purpose of this paper is to illustrate how the methods illustrated in the previous section for binary systems can be extended to ternary systems. Feed flowrate does not have to be considered because, even in multicomponent systems, changing all flows (reflux, vapor boilup, distillate, and bottoms) directly with feed flowrate maintains the same compositions and temperatures on all trays and maintains both product purities. Therefore, feed composition is the factor that must be dealt with.

Of course, in a ternary system, there are three components; so, two mole fractions are required to define the composition of a stream. In a binary system, a single feed composition z is varied. Now, two feed composition are varied. So, the "lines" that are generated in the "constant-purity" plots for a binary system now become "constant-purity surfaces" in a three-dimensional space.

The benzene/toluene/*o*-xylene ternary system is used as a numerical example. The feed is 1 kmol/s of a ternary mixture of 30 mol % benzene, 30 mol % toluene, and 40 mol % *o*-xylene. The column is designed to separate benzene from the other two heavier components. So, benzene is the light key component, and toluene is the heavy key component.

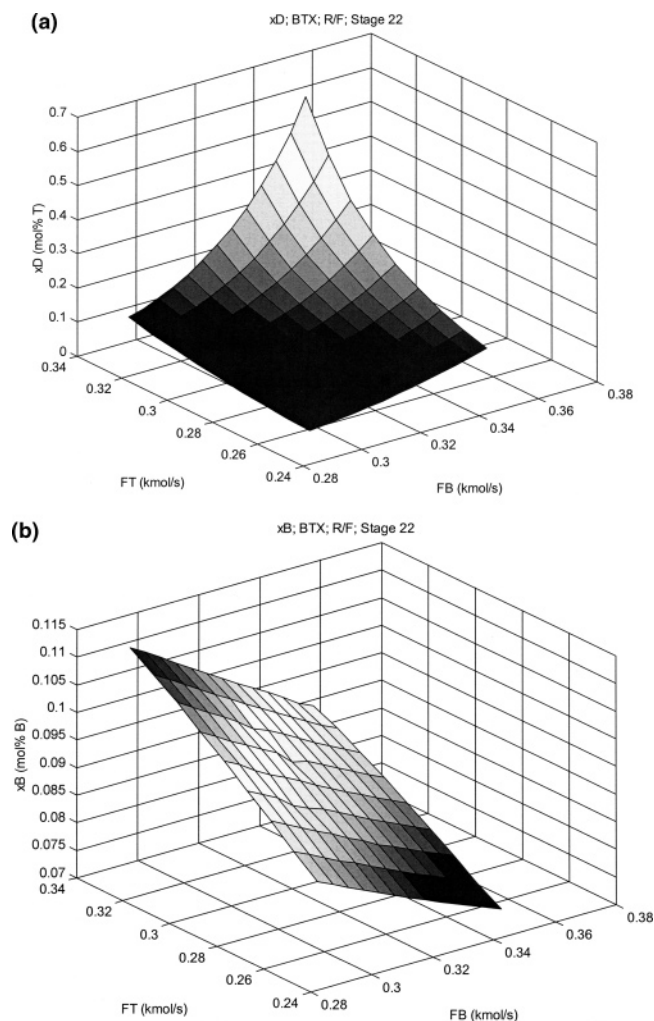


Figure 3. (A) x_D impurity for fixed R/F and Stage 22 temperature. (B) x_B impurity for fixed RR and Stage 22 temperature.

A 32 stage column is fed on Stage 16, which is the stage that minimizes reboiler heat input for the design feed composition. The column operates at 1 atm and produces high-purity products. The specified product impurities are 0.01 mol % toluene in the distillate and 0.01 mol % benzene in the bottoms. At the design feed composition ($z_B = 0.3$ and $z_T = 0.3$), the reflux ratio is 1.89 and the reflux-to-feed ratio is 0.565. Reboiler heat input is 42.0 MW, and the column diameter is 7.8 m.

A. Constant-Purity Surfaces. The purities of both products are held constant by using the "Design Spec-Vary" feature in Aspen Plus. The distillate-to-feed ratio and the reflux ratio are varied.

The molar flowrates of toluene and *o*-xylene are fixed, and the molar flowrate benzene is varied around the design value of 0.3 kmol/s using the "Sensitivity" feature in Aspen Plus. For each value of benzene flowrate, the required values of RR and R/F are stored. Then, new values of the molar flowrates of toluene and *o*-xylene are selected, and the calculations are repeated. The sum of the toluene and *o*-xylene molar flowrates is kept constant at 0.7 kmol/s.

The results are plotted in two three-dimensional spaces. Figure 2A shows how the reflux-to-feed ratio must change as the molar flowrates of the components change (which are equivalent to changes in feed compositions). Figure 2B shows how the reflux ratio must

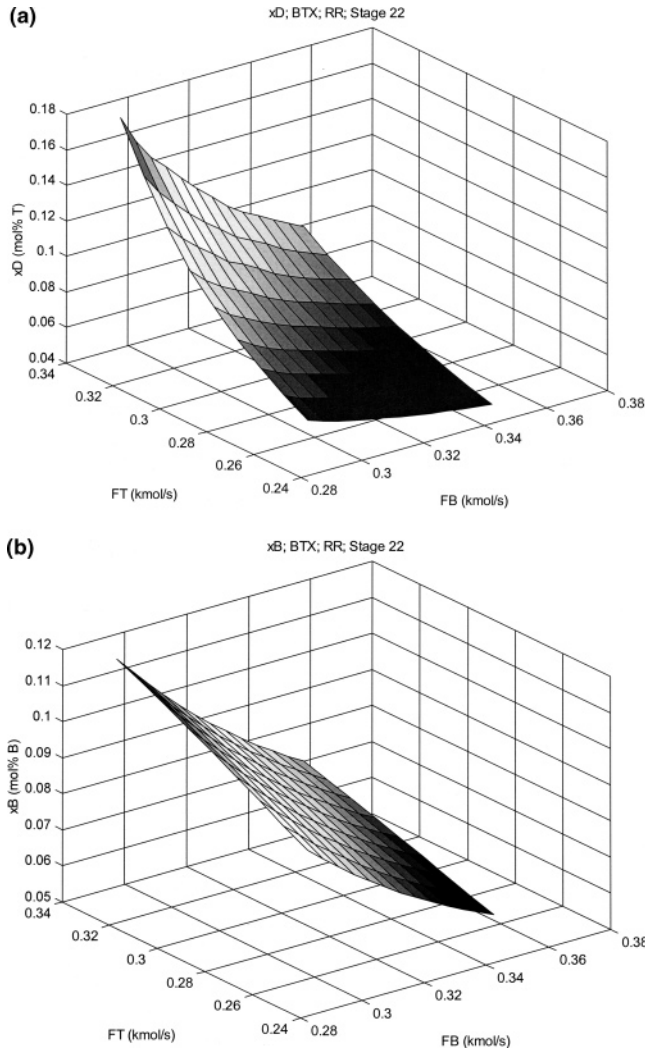


Figure 4. (A) x_D impurity for fixed RR and Stage 22 temperature. (B) x_B impurity for fixed RR and Stage 22 temperature.

change. Neither of these surfaces is very flat. This indicates that using either of these strategies in a single-temperature control structure may not be effective in this high-purity ternary system if feed composition disturbances occur.

B. Constant Tray Temperature and RR or R/F Surfaces. Other steady-state calculations can give additional insight into how well a given control structure will perform. Instead of holding product purities constant, a tray temperature and either RR or R/F are held constant by using the “Design Spec-Vary” feature. The resulting product purities are calculated over a range of feed compositions.

Figure 3 shows what happens to product impurities x_D and x_B when the temperature of Stage 22 is fixed and the reflux-to-feed ratio is held constant. The reason for selecting Stage 22 is discussed in the next section. The changes in product impurities are quite large for this structure, particularly in the distillate. This is expected because a temperature in the stripping section is being controlled, which is closer to the bottoms product.

Figure 4 shows what happens to product impurities x_D and x_B when the temperature of Stage 22 is fixed and the reflux ratio is held constant. The changes in product impurities are not as large for this RR structure

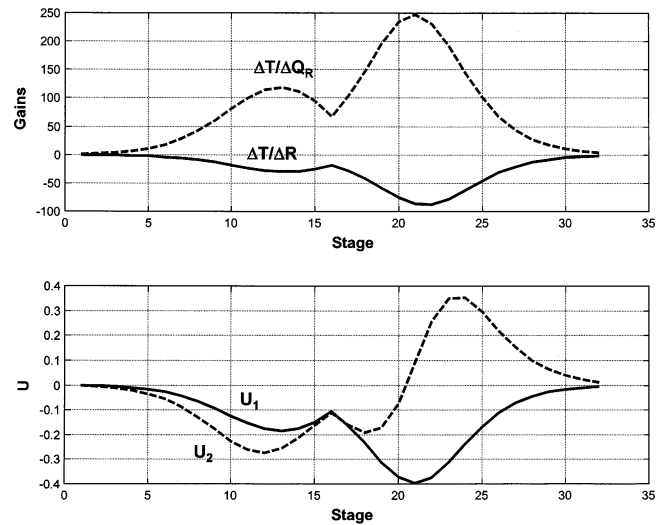


Figure 5. Steady-state gains and U vectors.

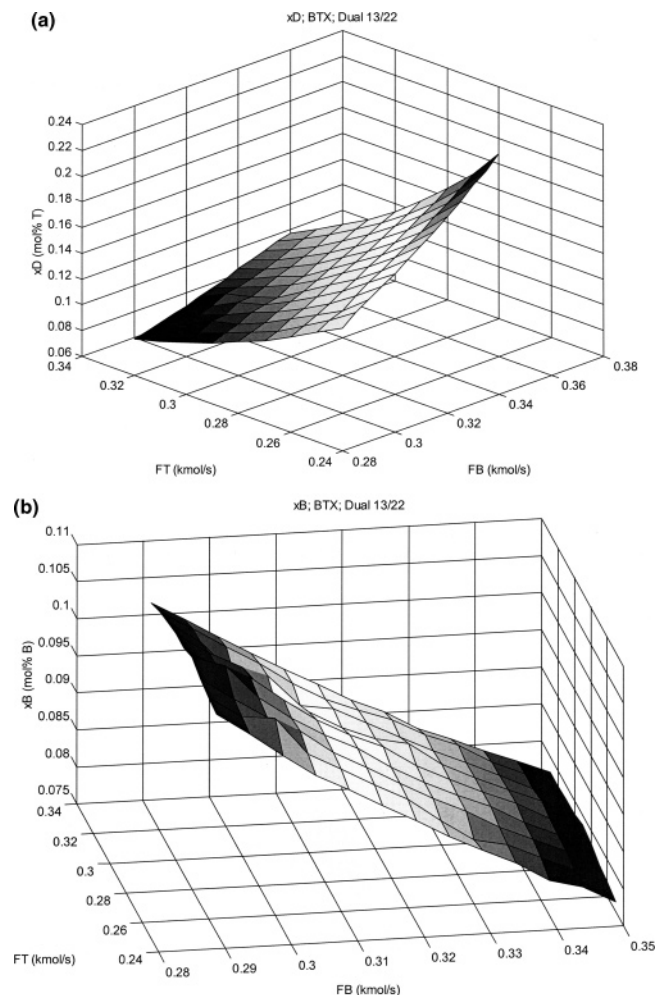


Figure 6. (A) x_D impurity for dual temperature control, Stages 13 and 22. (B) x_B impurity for dual temperature control, Stages 13 and 22.

as they are for the R/F structure. This suggests that the RR structure should give better performance from a steady-state perspective. However, product compositions vary quite a bit in both structures. This suggests that a dual temperature control structure may be required.

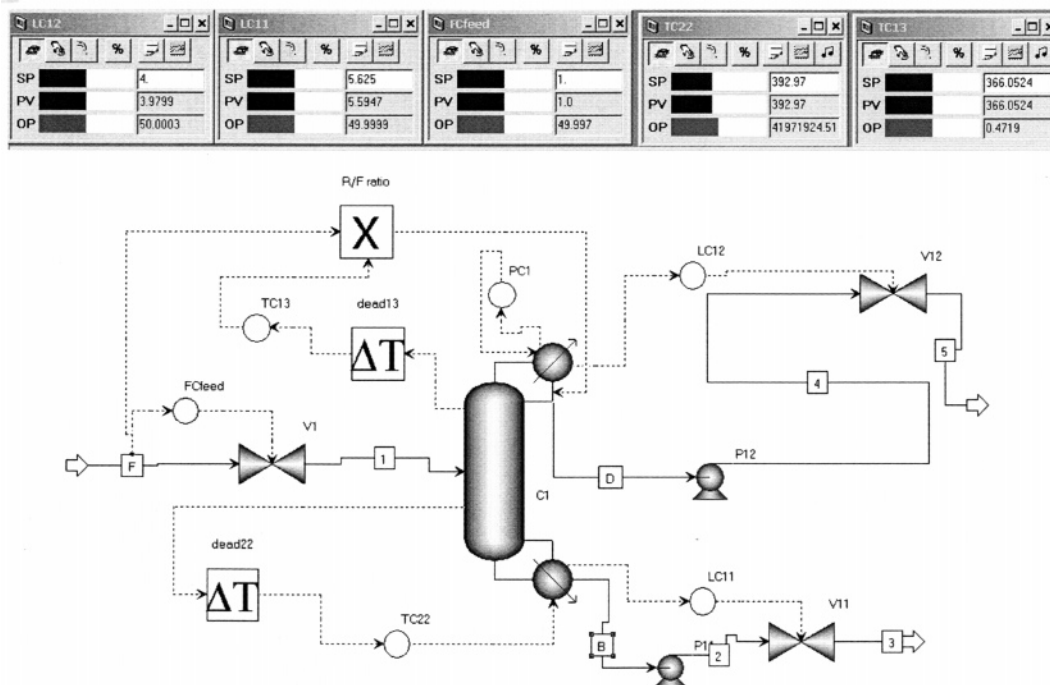


Figure 7. Dual temperature control structure.

4. Dual Temperature Control

A. Singular Value Decomposition (SVD). The selection of what tray or trays to control in a single or dual temperature control structure has an important impact on its effectiveness. Picking a tray where the temperature profile is the steepest in the column (most change in temperature from tray to tray) is usually quite reliable in a single temperature control structure. For a dual temperature control structure, the selection of two trays is more difficult. SVD methods provide useful guidance.

The steady-state gain matrix relating all the tray temperatures to the two manipulated variables (reflux and reboiler heat input) must be found. These gains can be found numerically using the steady-state simulator. Two runs are required, one for each of the inputs. A very small change (0.01% of the steady-state value) is made in the reflux flowrate 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 tray temperature and reflux. Then, the procedure is repeated for a very small change in the reboiler heat input with the reflux flowrate fixed.

These steady-state gains are shown in the upper graph in Figure 5. The dashed curves are for changes in reboiler heat input Q_R . The solid curves are for changes in 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 5. The peaks in the U curves indicate the most sensitive stages from a steady-state standpoint. Stages 13 and 22 are located near the peaks.

The magnitudes of the R peaks at Stage 22 are larger than those at Stage 13, which suggests the T_{22}/R

pairing. However, this is also true for the Q_R peaks. Remember that SVD is a steady-state analysis tool. It does not consider dynamics. Since controlling a tray higher in the column with reflux is faster than a tray that is lower, we select reflux to control the temperature of Stage 13 near the top of the column and reboiler heat input to control the temperature of Stage 22 near the bottom. Note that the Stage 13 controller is direct acting and the Stage 22 controller is reverse acting.

B. Steady-State Effectiveness. To assess the effectiveness of the dual temperature control structure to handle feed composition disturbances, the temperatures of Stages 13 and 22 are fixed using the Design Spec/Vary feature. Changes are made in feed composition in two dimensions, and the resulting product purities are plotted in three-dimension plots.

Figure 6A and B show how the impurities in the distillate and bottoms products vary as feed composition changes. The variability is much less than when either of the single temperature control structures are used.

C. Dynamics. Up to this point, we have considered only the steady-state aspects of the problem. It is vital that the dynamic controllability also be assessed. The flowsheet is exported in Aspen Dynamics after specifying column diameter and liquid holdups in the base and reflux drum. These, as sized to provide 5 min of holdup when half full, are based on total liquid entering or leaving the surge volume.

The dual temperature control structure is shown in Figure 7. Stage 22 temperature is controlled by manipulating reboiler heat input. Reflux is ratioed to feed, with the ratio being set by the Stage 13 temperature controller. Both temperature loops have 1 min dead-times. Temperature transmitter spans of 100 K are used.

This interacting system is tuned using a sequential approach that takes interaction explicitly into account. First, the faster of the two loops is tuned, which is the

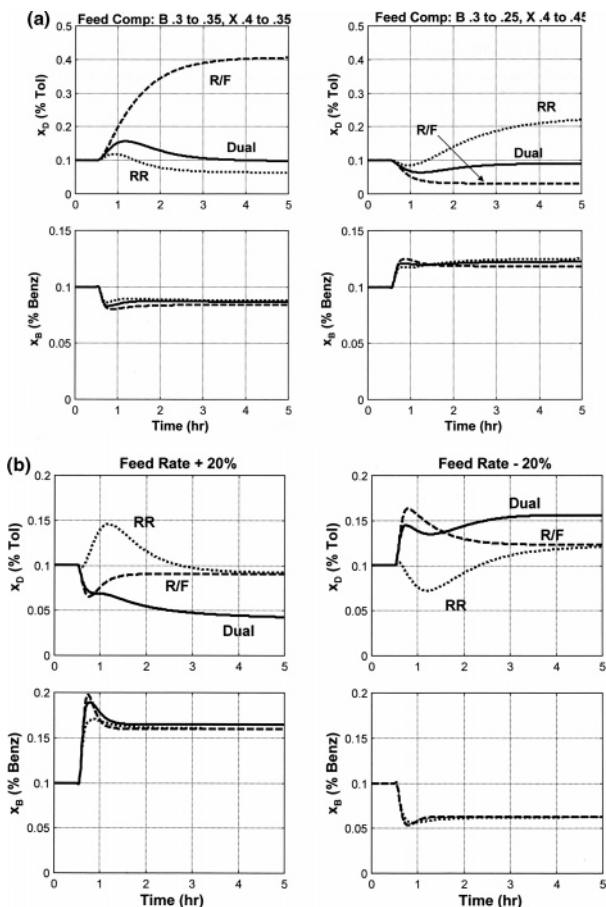


Figure 8. (A) Dual temperature control; feed composition changes. (B) Dual temperature control; feed rate changes.

T_{22}/Q_R loop. A relay-feedback test gives the ultimate gain and period, and the Tyreus-Luyben¹⁰ tuning equations give $K_C = 3.0$ and $\tau_I = 9.2$ min. This loop is placed on automatic, and the T_{13}/R loop is tuned in the same way. The resulting controller constants are $K_C = 4.1$ and $\tau_I = 25$ min. Note that the reflux loop is considerably slower than the heat input loop.

The effectiveness of the dual temperature control structure is demonstrated in Figure 8 where a direct comparison is given with the two single temperature control structures (RR and R/F). Figure 8A gives the product impurity level for two different feed composition disturbances. The left graphs are when the benzene composition of the feed z_B is changed from 30 to 35 mol % while the *o*-xylene composition of the feed z_X is changed from 40 to 35 mol %. The solid lines are for dual temperature control, the dashed lines are for R/F with Stage 22 control, and the dotted lines are for RR with Stage 22 control. For this disturbance, the dual temperature and the RR structures work well, but the R/F structure produces a large increase in the impurity of the distillate product x_D .

The right graphs are when the benzene composition of the feed z_B is changed from 30 to 25 mol %, while the *o*-xylene composition of the feed z_X is changed from 40 to 45 mol %. Now, the RR control structure results in a fairly large increase in the toluene impurity in the distillate.

Note that the dual temperature control structure does not give perfect control of product purities. But, it is significantly better than either of the single temperature

structures. Of the two, the reflux ratio structure is better. Note that we demonstrated earlier that the opposite is true for the binary benzene/toluene separation.

Figure 8B gives responses of the three alternative control structures for positive and negative 20% step changes in feed flowrate. The interesting aspect of these results is that the compositions of the products do *not* return exactly to their original values. We stated earlier that feed rate changes can be handled by any of the schemes because all flows change directly with the feed flowrate. But, we see in Figure 8B that this is not the result.

The explanation for this is the change in pressure drop through the column as vapor boilup changes in the dynamic Aspen Dynamic model. This results in a different composition on the control tray for the same temperature. It should be noted that this effect is not seen in the steady-state results obtained from Aspen Plus, since the tray pressure drop is specified by the user and does not change for different vapor rates. This illustrates one of the several subtle differences that exist between steady-state Aspen Plus and dynamic Aspen Dynamics.

It should be pointed out that it is sometimes useful to include dynamic lags in the reflux-to-feed ratio. Some of the transient peaks in the results shown in Figure 8B could be reduced with suitable dynamic elements.

5. Conclusion

This paper has demonstrated how the steady-state analysis for binary distillation columns can be extended to ternary systems. The constant-purity curves for binary systems become constant-purity surfaces for ternary system.

This steady-state analysis provides guidance in selecting between single temperature control and dual temperature control. It also aids in choosing between holding reflux ratio constant or holding reflux-to-feed ratio constant.

Nomenclature

- F = feed flowrate (kmol/s)
- F_B = molar flowrate of benzene in feed (kmol/s)
- F_T = molar flowrate of toluene in feed (kmol/s)
- F_X = molar flowrate of *o*-xylene in feed (kmol/s)
- R = reflux flowrate (kmol/s)
- R/F = reflux-to-feed ratio
- RR = reflux ratio = R/D
- T_n = temperature on stage n (K)
- x_B = impurity in bottoms product (mf benzene)
- x_D = impurity in distillate product (mf toluene)
- z_B = composition of feed (mf benzene)
- z_T = composition of feed (mf toluene)
- z_X = composition of feed (mf *o*-xylene)

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