19 Calculation of Steady-State Gains

19.1 INTRODUCTION

Most composition control schemes for a binary column involve manipulating either reflux or distillate to control top composition, and either boilup or bottom product to control bottom composition. Changes in either of the two top manipulative variables will affect not only top composition, but bottom composition as well. Correspondingly, changes in either bottom-product flow or boilup will affect both bottom and top compositions. As a minimum, therefore, for feedback control purposes we are interested in two composition gains at each end of the column.

The calculations to predict how a column already designed or built will operate are intrinsically more difficult than are column design calculations. As pointed out in a paper by Douglas and Seemann, "The number of plates required to achieve a given separation at a specified reflux ratio can be calculated directly, but is implicit in terms of the control variables, i.e., the reflux rate required to achieve a given separation if the number of plates is specified must be obtained by trial-and-error procedures." An appreciation of the labor required may be obtained by a perusal of papers such as those of Uitti, and Bauer and Orr, who made trial-and-error use of McCabe–Thiele diagramming. More recently Wood used a digital computer for trial-and-error calculations via the tray-to-tray method, while Buckley, Cox, and Luyben performed similar calculations on a programmable calculator.

Other workers in the field seem primarily interested in such calculations to determine the economic penalty of either overrefluxing (via excess boilup) or of specifying product purities better than needed. To obtain column gains, we need go only one step further. For example, it is only necessary to make a number of top and bottom composition calculations for different reflux ratios, plot the points of top and bottom purities versus reflux ratio, and draw curves
through the points. Then the slope of either curve is the “gain” of top or bottom composition as a function of reflux ratio.

Some workers have used the Smoker analytic method rather than the tray-to-tray method. The former has the disadvantage of requiring the assumption of constant relative volatility but has the advantage of being much faster when programmable calculators or small computers are used. However, the tray-to-tray method easily handles relative volatility as a function of composition, and reads out any or all tray compositions. We feel that the advantages of the tray-to-tray method outweigh the disadvantage of longer run times.

Most industrial columns are not binary and do not have constant relative volatility from top to bottom. Two fundamental problems therefore confront the engineer at the outset:

1. How to make a reasonable binary approximation of a multicomponent column. Such an approximation greatly reduces computation and time.
2. How to derive a relationship between liquid composition on each tray and relative volatility.

As is shown here, the second problem must be dealt with first. The following procedure is suggested:

1. Pick a light key and a heavy key—or a low boiler and a high boiler.
2. Using printouts of multicomponent design calculations, calculate mol fraction low boiler, $x_{LB}$, on a binary basis and relative volatility at each tray.
3. Use curve-fitting techniques to relate $x_{LB}$ and relative volatility at each tray.
4. Go through binary design calculations to check the total number of theoretical trays and feed-tray location. If the match with the multicomponent calculations is not adequate, go to step 3 and use a higher order function for curve fitting.

The basic approach then consists of defining a base case, usually the design case, to firm up feed-tray location (number of trays above and below the feed tray), reflux ratio, and boilup ratio. With these in hand, we may calculate the effect of changing reflux ratio, and so forth.

19.2 DESIGN PROCEDURE

Since we will use the tray-to-tray method, it is appropriate to begin by stating the required assumptions:

1. Simple column with a single feed and top- and bottom-product drawoffs.
2. Binary or pseudobinary separation. As shown by Strangio and Treybal, surprisingly good accuracy can be obtained in many cases by approximating a multicomponent system as a binary system. Sometimes a multicomponent system
can be modeled as one binary in the bottom section and as a different binary in the upper section.

3. Equimolar overflow.

4. One top product that is all liquid.

5. One bottom product that is all liquid.

6. Feed that may be single-phase vapor or liquid, or may be mixed phase in nature.

7. Partial reboiler and total condenser.

In the first programmable calculator programs we developed, three choices were available for relative volatility: (1) constant, (2) a linear relationship between $\alpha$ and liquid composition $x$, and (3) a quadratic relationship between relative volatility and liquid composition on a tray. But the first time we tried these on a real column for MeOH-H$_2$O, it proved inadequate. We now have an HP-41C program that fits a quadratic to each of six segments of a column to relate relative volatility and tray number.

The design program (see also Chapter 2) starts with data provided by the column designer or plant. This includes feed flow rate, composition, and enthalpy or $q$. It also includes top- and bottom-product compositions and reflux ratio, $L_R/D$. Running a design program is not absolutely necessary for our purposes, but it is one way of initializing subsequent programs and of checking assumptions. The following steps are involved.

1. Find:

$$\beta = \frac{V_s}{B}$$ (19.1)

$$\beta = \frac{R(z_F - x_B) + q(x_D - x_B) - (x_D - z_F)}{(x_D - z_F)}$$ (19.2)

2. Find:

$$y_i = \frac{(\beta + 1)x_D + Rx_B}{(\beta + 1) + R}$$ (19.3)

This is the $y$ corresponding to the intercept of the operating and $q$ lines. For optimum design it is also the composition of vapor above the feed tray.

3. The tray-to-tray calculations come next. If trays are numbered from the top down, it is customary to start at the top. If trays are numbered from the bottom up, the base is the usual starting point. We will follow the second practice.

3.1 Starting at the column base and working upward, find:

$$y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n}$$ (19.4)

This is the equation defining the vapor–liquid equilibrium relationship.
It is the $x$ versus $y$ curve for a McCabe–Thiele diagram. Note that the first $x$ is $x_B$.

3.2 Find:

$$x_{n+1} = \frac{\beta y_n + x_B}{\beta + 1} \quad (19.5)$$

This is the material-balance equation and its initial application gives $x_1$, liquid composition on the bottom tray.

3.3 Repeat 3.1, using $x_1$ to calculate $y_1$. Then use $y_1$ in 3.2 to calculate $x_2$, and so on until $y \geq y_i$. The number of times that we perform 3.1 [equation (19.4)] is $N_s$, the number of stages there are in the stripping section, including feed tray and the reboiler (assuming there is one). The number of times that we perform 3.2 [equation (19.5)] is one less, and therefore represents the number of theoretical trays, including the feed tray.

4. Starting with the tray above the feed tray, we switch operating lines.

4.1 Find:

$$x_{n+1} = \frac{(R + 1)y_n - x_D}{R} \quad (19.6)$$

This is the material-balance equation for the rectification section. The first $x$ calculated is that of the first tray above the feed tray; the value of $y$ used is that of the feed tray.

4.2 Find:

$$y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n} \quad (19.7)$$

4.3 Repeat 4.1 and 4.2 until $y \geq x_D$ (total condenser assumed). The number of times 4.1 and 4.2 have been repeated is $N_R$, the number of stages in the rectification section. Since the condenser is assumed to be a total condenser, it does not count as a stage. A partial condenser would count as a stage.

19.3 EXACT $R$ PROCEDURE

The "design" program usually leads to a design that produces top-product purity slightly better than specification for an integral number of trays (if we start at the top instead of the bottom, it produces bottom-product purity slightly better than specification). What we need to do next is to find a slightly different, "exact" value of $R$ that causes the column to produce top and bottom purities that exactly match specifications. This may be determined by the following procedure, designated "Type A":

1. Assume a new value of $R$ slightly smaller than that used for design.
2. Calculate $\beta$ from equation (19.2).
3. Starting at the column base and working upward, find:

\[ y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n} \]  \hspace{1cm} (19.4)

\[ x_{n+1} = \frac{\beta y_n + x_B}{\beta + 1} \]  \hspace{1cm} (19.5)

Repeat until the number of times equation (19.4) has been used equals \( N_f \).

4. Use the \( y \) thus calculated for the feed tray. Then switch operating lines and find:

\[ x_{n+1} = \frac{(R + 1)y_n - x_D}{R} \]  \hspace{1cm} (19.6)

\[ y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n} \]  \hspace{1cm} (19.7)

If the calculated \( x_{n+1} < x_n \), assume a slightly larger value of \( R \) and start again at step 1. As indicated by Figure 19.1, we must be careful to provide program logic to prevent “taking off” to the left of the equilibrium curve.

5. Repeat equations (19.6) and (19.7) until they have been used \( N_T - N_s = N_R \) times.

6. Compare last \( y = y_T \) with specified \( x_D \). If \( y_T \) does not match within a preselected tolerance, go back to step 1, assume a new value of \( R \), and repeat steps 2–6.

A number of convergence procedures are available for step 6. We have, for example, used a simple “proportional controller,” that is, we multiply the “error” \( y_T - x_D \) by a constant with the proper polarity for negative feedback. This requires some trial and error to achieve a balance between oscillation and excessively slow response. A better method is a modified interval-halving technique that provides moderately rapid convergence without instability.

Originally we used 0.0002 as a tolerance: \( |y_T - x_D| \). This proved to be too large for some purposes so we switched to \( 10^{-7} \).

### 19.4 COLUMN OPERATION PROCEDURE

Many different modes of column operation and control can be visualized, but for preparing programs, we must keep in mind at least four needs:

1. Column gains for feedback control. Here, for example, we need to know the change in top composition due to a change in distillate or reflux flow with other variables held constant.

2. Column terminal composition sensitivity to changes in feed rate, feed enthalpy, feed composition, and column pressure (usually defined at column
Figure 19.1
Effect on calculation of rectifying section when:
A. Guess for $R$ is too small, or
B. Guess for $x_0$ is too close to 1.00000
overhead). These sensitivities often give good clues to the need for feedforward compensation or for terminal composition feedback control.

3. Column gains for feedforward compensation. For example, if feed composition changes, what changes in boilup and reflux do we need to hold terminal compositions constant? Steady-state accuracy is required.

4. Ability to estimate the cost penalty of producing excessively pure product by excessive boilup and reflux. Shinskey and Douglas and Seemann have been particularly interested in this. Again, steady-state accuracy is required.

As it turns out, for most of these concerns, we use one of two types of programs: (1) Column terminal conditions are fixed at new, different values from those of design, and reflux is varied by trial and error until the material-balance equation and tray-to-tray calculations converge, or (2) with fixed reflux or boilup, we change a terminal condition such as distillate flow and find the corresponding change in terminal compositions. The first of these we have labeled "Type A" and the second we call "Type B."

Gains for Feedback Control

Consider Figure 19.2 where top-product flow is set by flow control, reflux flow is set by condensate receiver level control, boilup is fixed by flow control of steam or other heating medium, and bottom-product flow is determined by column-base level control. As shown by the dotted line, we wish eventually to control column top composition by manipulating distillate flow. Let us assume that feed rate, feed composition, feed enthalpy, and boilup are fixed and that we wish to find the changes (i.e., "gains") of top and bottom compositions in response to a change in \( D \), the top-product rate.

The starting point is a set of "prep" equations that reflect the desired change in distillate, \( \Delta D \). The new distillate flow is:

\[
D' = D + \Delta D
\]

and

\[
B' = B - \Delta D \quad \text{(since } F \text{ is fixed at 1.00)}
\]

\[
\beta' = V'/B'
\]

\[
L_R = L_R - \Delta D
\]

\[
R' = L_R/D'
\]

1. With these equations in hand, assume a new value of \( x_D = x'_D \) and calculate a new \( x'_B \):

\[
x'_B = z_F + \frac{D'}{B'} (z_F - x'_D)
\]
2. Calculate:

\[ y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n} \]

starting at the column base and working up.

3. Calculate:

\[ x_{n+1} = \frac{\beta' y_n + x'_B}{\beta' + 1} \]

Continue calculating \( y \) and \( x \) alternately until the number of times \( y \) has been calculated equals \( N_f \).

FIGURE 19.2
Reflux via reflux drum level control; bottom product via base level control
4. Switch to rectification operating line.
4.1 Calculate:

\[ x_{n+1} = \frac{(R' + 1)y_n - x'_D}{R'} \]

and

\[ y_n = \frac{\alpha x_n}{1 + (\alpha - 1)x_n} \]

4.2 If the first calculated \( x \) shows that \( x_k < x_{k-1} \) (Figure 19.1), assume a new and larger value of \( x_B \) and resume at step 4. Continue until \( N = N_T - N_S = N_R \).

5. Determine when the calculation is complete, that is, when the estimated \( x_B^* \) is equal to \( y \) at the top tray. If \( |y_T - x_D| \) is greater than the chosen tolerance, choose new \( x_B^* \) and repeat steps 1–5.

Note that changing \( B \) is equivalent for this case to changing \( D \). We will term the procedure for steps 1–5 the Type B procedure in contrast to the Type A procedure.

The reader may have observed that although we need only the change in \( x_D \) for a change in \( D \) to design the overhead composition control system, we have also calculated the change in \( x_B \) in response to a change in \( D \). This second gain is an interaction term. Note that we call the preceding Type B.

Since the original design calculations are unconverged, it is necessary, when the Type B program is to be used, first to obtain converged values of \( x_B \) and \( x_D \) for the specified reflux and boilup.

Case 2

If we desire to control bottom composition by changing boilup as shown on Figure 19.2, we would start by assuming that both feed and top-product rates are fixed. This means that bottom product is also fixed. The "prep" equations for ultimately finding new base composition, \( x_B' \), and new top composition, \( x_D' \), are therefore:

\[ V' = V + \Delta V \]
\[ L' = L + \Delta V \]
\[ \beta' = V'/B \]
\[ R' = L'/D \]

Then use the Type B routine.

To control base composition via boilup, we need the gain of \( x_B \) with respect to \( V' \). The second gain, change in \( x_D \) with respect to \( V' \), is another interaction term. The magnitudes of the interaction terms give clues to the need for decouplers.
Another commonly encountered control scheme is that of Figure 19.3. This is similar to that of Figure 19.2 except that overhead condensate receiver level is controlled by throttling distillate, while reflux is flow controlled, perhaps eventually cascaded from top composition control.

If feed and boilup are fixed at design conditions, top and bottom composition $x'_D, x'_B$ response to reflux changes may be found by starting with the following “prep” equations:

\[
\begin{align*}
L_R &= L_R + \Delta L_R \\
B' &= B + \Delta L_R \\
\beta' &= V_s/B' \\
D' &= D - \Delta L_R \\
R' &= L_R/D'
\end{align*}
\]

**FIGURE 19.3**
Distillate via reflux drum level control; bottom product via base level control
The Type B routine, described in the discussion of Case 1, would then be required.

Note that if the original design calculations were done on the assumption that reflux is not subcooled, the effect of subcooling may be considered as a change in $L_R$:

$$\Delta L_R = \frac{c_p}{\lambda} (T_o - T_R)$$

If the base case assumes some subcooling ($T_R = T_{R1}$), and later the subcooling is different ($T_R = T_{R2}$):

$$\Delta L_R = \frac{c_p}{\lambda} (T_{R2} - T_{R1})$$

**Case 4**

For the control system of Figure 19.3, if feed and reflux are fixed, and if it is desired to find the responses $x_D$, $x_B$ to changes in boilup, the following "prep" equations are required:

$$B' = B - \Delta V_s$$
$$V_s' = V_s + \Delta V_s$$
$$\beta' = V_s'/B'$$
$$D' = D + \Delta V_s$$
$$R' = L_R/D'$$

The Type B routine, described in discussion of Case 1, is then required.

**Case 5**

A third basic control scheme is that of Figure 19.4. Here overhead condensate receiver level is controlled by throttling distillate flow, while reflux is flow controlled, perhaps ultimately cascaded from overhead composition control. Base level is controlled by adjusting heating-medium flow control. Bottom-product flow is on flow control, perhaps ultimately cascaded from bottom-product composition control.

If feed and bottom rates are fixed, we wish to find the responses $x_D$, $x_B$ to a change in reflux flow. The following "prep" equations are required:

$$L_R' = L_R + \Delta L_R$$
$$V_s' = V_s + \Delta L_R$$
$$\beta' = V_s'/B$$
$$R' = L_R/D$$

The Type B routine, described in the discussion of Case 1, is required.
If, for Figure 19.4, feed and reflux are fixed, we may wish to find the responses $x'_D, x'_B$ to a change in bottom-product flow. The following “prep” equations are required:

\[
\begin{align*}
B' &= B + \Delta B \\
V'_t &= V_t - \Delta B \\
\beta' &= V'_t / B' \\
D' &= D - \Delta B \\
R' &= L_R / D'
\end{align*}
\]

The Type B routine, described under Case 1, is required.

**FIGURE 19.4**
Distillate via reflux drum level control; boil up via base level control
Column Terminal Composition Sensitivity to Various Inputs

Case 7

For the control system of Figure 19.2, we may wish to determine overhead and base composition responses to changes in feed rate. The following “prep” equations are needed:

$$B' = \frac{B + \Delta F}{1 + \Delta F}$$
$$\beta' = \frac{V_f}{B'}$$
$$L'_R = L_R + (1 - q)\Delta F$$
$$D' = 1 - B'$$
$$R' = \frac{L'_R}{D'}$$

In the first equation above, $B'$ might better be labeled $B''$. Since $D$ is fixed:

$$B' = B + \Delta F$$

But our program requires that all flows be relative to $F = 1$. Therefore let:

$$B' = \frac{B + \Delta F}{F + \Delta F} = \frac{B + \Delta F}{1 + \Delta F}$$

For simplicity of symbolism, we represent $B''$ by $B'$.

Case 8

For the control system of Figure 19.2, we may wish to find the responses $x_b'$ and $x_b$ to changes in $q$. The following “prep” equations are needed:

$$q' = q + \Delta q$$
$$L'_R = L_R - (\Delta q)F$$
$$R' = \frac{L'_R}{D}$$

Use the Type B program as described under Case 1.

Case 9

For the control system of Figure 19.3, we may wish to determine overhead and base composition responses to changes in feed rate. The following “prep” equations are needed:

$$B' = \frac{B + q\Delta F}{1 + \Delta F}$$
$$\beta' = \frac{V_f}{B'}$$
$$D' = 1 - B'$$
$$R' = \frac{L_R}{D'}$$
In the first equation above, $B'$ again might more properly be written $B''$. For a change in $F$ to $F' = F + \Delta F$:

$$B' = L_R + q(F + \Delta F) - V,$$

But:

$$B = L_R + qF - V,$$

and therefore:

$$B' - B = q\Delta F$$

or

$$B' = q\Delta F + B$$

Since our programs are based on 1 mole feed per unit time, let us define:

$$B'' = \frac{q\Delta F + B}{F + \Delta F}$$

$$B'' = \frac{q\Delta F + B}{1 + \Delta F}$$

Again, for simplicity of symbolism, we use $B'$ instead of $B''$. A Type B program, discussed under Case 1, should be used.

**Case 10**

For the control system of Figure 19.3, we may wish to find the responses of $x_D$ and $x_B$ to changes in $q$. The following “prep” equations are required:

$$q' = q + \Delta q$$

$$B' = B + (\Delta q)F$$

$$\beta' = V_s/B'$$

$$D' = D - (\Delta q)F$$

$$R' = L_R/D'$$

The Type B program (see Case 1) should then be employed.

**Case 11**

For the control system of Figure 19.4, we may wish to determine overhead and base composition responses to changes in feed rate. The following “prep” equations are required:
\[ B' = \frac{B}{1 + \Delta F} \]
\[ V'_i = V_i + q\Delta F \]
\[ \beta' = \frac{V'_i}{B'} \]
\[ D' = 1 - B' \]
\[ R' = \frac{L_R}{D'} \]

Use the Type B program (see Case 1).

**Case 12**

For the control system of Figure 19.4, we may wish to determine overhead and base composition responses to changes in feed enthalpy factor, \( q \). The following “prep” equations are needed:

\[ q' = q + \Delta q \quad F = 1.00 \]
\[ V'_i = V_i + (\Delta q)F \]
\[ \beta' = \frac{V'_i}{B} \]

Use the Type B program (see Case 1).

**Case 13**

For any of the control schemes, the effect of feed composition change from \( z_F \) to \( z'_F \) on \( x_D \) and \( x_B \) may be found simply by entering the new \( z'_F \) into data storage for the Type B program (see Case 1).

**Case 14**

For any of the control schemes, the effect of a column pressure change from \( P \) to \( P' \) on \( x_D \) and \( x_B \) may be found by recalculating \( \alpha \)'s; rerunning the program for the quadratic coefficients \( A, B, \) and \( C \); and entering the new values of \( A, B, \) and \( C \) in the Type B program (see Case 1).

**Column Gains for Feedforward Compensation**

Here the objective is to find required feedforward compensator gain to hold terminal composition constant as various external factors vary.

**Case 15**

For any of the control systems discussed—Figure 19.2, 19.3, or 19.4—assume that top composition and bottom composition are held constant. We wish to find the changes in \( L_R, D, B, \) and \( V \), required to hold compositions constant in the face of a feed composition change, \( \Delta z_F \). This information could be used to design feedforward compensators to minimize transient changes in terminal compositions. The variables chosen for feedforward compensation will depend on which feedback control scheme is used—Figure 19.2, 19.3, or 19.4.
The equations required to recalculate the other variables are:

\[ z'_F = z_F + \Delta z_F \quad F = 1.00 \]

\[ D' = D + \frac{F \Delta z_F}{x_D - x_B} \]

\[ B = F - D' \]

Use the Type A program, described in Section 19.3.

**Case 16**

This is the same as Case 15 except that \( q \) is changed. The only equation needed is:

\[ q' = q + \Delta q \]

Use the Type A program (see Section 19.3).

**Case 17**

This is the same as Case 15 except that column top pressure is changed to \( P' = P + \Delta P \). Relative volatilities should be recalculated and the quadratic coefficients \( A_n, B_n, \) and \( C_n \) reevaluated. Then run the Type A program (see Section 19.3).

**Economic Penalty of Overrefluxing**

**Case 18**

If product purity at one end of the column, say \( x_D \), is set at a new, constant, higher value, to ensure that product purity is always at least as good as the original specification, we may wish to estimate the cost penalty of the increase boilup. We will need to know \( L_R \) and \( V_r \). If the column control scheme fixes either \( D \) or \( B \), the other will also be fixed. Then if one new terminal composition is chosen, the other is readily calculated:

\[ x'_D = x_D + \Delta x_D \]

\[ x'_B = x_B - x_D \left( \frac{D}{B} \right) \]

Use the Type A program (see Section 19.3).

**Case 19**

If we have a situation similar to that of Case 18 except that both a new \( x'_D \) and a new \( x'_B \) are chosen, we will get changes in \( D \) and \( B \) as well as \( L_R \) and \( V_r \):

\[ x'_D = x_D + \Delta x_D \quad B'/F' = \frac{z_F - x'_D}{x'_B - x'_D} \]

\[ x'_B = x_B + \Delta x_B \quad D' = F - B' \]
19.4 Column Operation Procedure

Use the Type A program (see Section 19.3).

Shinskey⁷ has pointed out that the differences between the design value of \( V_i/F \) and those required for higher values of \( x_D \) are measures of the cost of overrefluxing.

**Case 20**

If a column has automatic control of \( R = L_R/D \) (it does not matter whether condensate receiver is level controlled via reflux or top product), the following “prep” equations apply for constant \( V_i \):

\[
\begin{align*}
R' &= R + \Delta R \\
L_R' &= R'D' \\
L_R' + D' &= L_R + D
\end{align*}
\]

or

\[
R'D' + D' = RD + D
\]

so:

\[
D' = \left(\frac{1 + R}{1 + R'}\right) D
\]

\[
B' = 1 - D'
\]

\[ \beta = V_i/B' \]

Use the Type B procedure (see Case 1).

**Case 21**

For a column with automatic control of \( R = L/D \), the following “prep” equations apply for constant \( R \):

\[
\begin{align*}
V_i' &= V_i + \Delta V_i \\
D' + L_R' &= V_R' = V_i (1 - q)
\end{align*}
\]

But:

\[ L_R' = RD' \]

so:

\[ D' + RD' = V_i' (1 - q) \]

or

\[
D' = \frac{V_i' (1 - q)}{1 + R}
\]

\[ 1 - D' = B' \]

\[ V_i'/B' = \beta' \]
Use the Type B procedure (see Case 1).

19.5 EXAMPLES

Example 1: Calculation of Column Gains

Let us use a test case where the following conditions apply:

\[ \begin{align*}
    z_F &= 0.46 \\
    x_D &= 0.98 \\
    x_B &= 0.01 \\
    q &= 0.7 \\
    \alpha &= 2.80 \text{ at } x = 0.20 \\
    \alpha &= 2.20 \text{ at } x = 0.80 \\
    R &= 2.50
\end{align*} \]

Our HP-97 program predicts:

\[ \begin{align*}
    N_r &= 7 \\
    N_T &= 16 \\
    N_R &= 9 \\
    \beta &= 2.469 \\
    (x_D)_{\text{final}} &= 0.9930
\end{align*} \]

Next we found the exact \( R \) to be 2.306. We then chose to find the column gains, \( \frac{dx_D}{dD} \) and \( \frac{dx_B}{dD} \), which is Case 1.

After running the design and exact \( R \) (Type A) cases, we made a data card. With this card, we ran a Type B program twice, once for \( D \) slightly smaller than design, and once for \( D \) slightly larger than design. \( V \) was held constant. We fitted the two sets of three points—one set for \( x_D \) and one set for \( x_B \)—to a quadratic function:

\[ y = Ax^2 + Bx + C \]

\[ \frac{dy}{dx} = 2Ax + B \]

The results are tabulated in Table 19.1. We arbitrarily chose \( F = 1.00 \), so for the design case, \( D = 0.46392 \) and \( B = 0.53608 \). Although we chose small changes, \( \Delta D = 0.001 \), we found large changes in gain with changes in \( D \). The gain is a very nonlinear function, decreasing as \( x_D \) increases and as \( D \) decreases. It is also a function of \( F \). One could use this information to design a suitable nonlinear or adaptive control scheme.
Example 2: Economic Penalty of Overrefluxing

Douglas and Seemann\(^1\) have investigated the consequences of overrefluxing a deisobutanizer. Design conditions were:

\[
\begin{align*}
z_F &= 0.575 \\
x_D &= 0.950 \\
x_B &= 0.050 \\
g &= 1.00 \\
\alpha &= 1.332 \\
R &= 5.87
\end{align*}
\]

They assumed a control system in which distillate is flow controlled, reflux is set by condensate receiver (reflux drum) level control, and bottom-product rate is controlled by column-base level. Overhead composition is controlled by boilup.

For the design case, Douglas and Seemann calculated by their analytical method, based on a simplified Smoker equation, that \(N_z = 26.30\) stages, including the reboiler, and \(N_R = 31.65\) trays. The exact Smoker equation, as well as the tray-to-tray method, predicts \(N_z = 21\) stages and \(N_R = 18\) stages. Predicted overhead composition by our HP-97 program is 0.9520. The exact \(R\) turns out to be 5.852. Again we made a data card at this point to minimize subsequent calculations.

Table 19.2 shows the results obtained with various values of \(x_D\) greater than the design value of 0.950.

<table>
<thead>
<tr>
<th>D</th>
<th>(x_D)</th>
<th>(x_B)</th>
<th>(\frac{dx_D}{dD})</th>
<th>(\frac{dx_B}{dD})</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.46292</td>
<td>0.98113</td>
<td>0.010835</td>
<td>-1.063</td>
<td>-0.891</td>
</tr>
<tr>
<td>0.46392</td>
<td>0.98000</td>
<td>0.01000</td>
<td>-1.189</td>
<td>-0.780</td>
</tr>
<tr>
<td>0.46492</td>
<td>0.97875</td>
<td>0.009273</td>
<td>-1.314</td>
<td>-0.670</td>
</tr>
</tbody>
</table>

Table 19.1: Variation of terminal compositions and gains with distillate rate for a constant boilup rate (gains on basis 1.00 mols feed)
### TABLE 19.2
Energy increase due to over-refluxing deisobutanizer

| TOP PRODUCT COMPOSITION $X_D$ | 0.950 | 0.955 | 0.960 | 0.965 | 0.970 |
| BOTTOM PRODUCT COMPOSITION $X_B$ | 0.050 | 0.043 | 0.036 | 0.029 | 0.022 |
| REFLUX RATIO $R = \frac{L_R}{D}$ TRAY-TO-TRAY | 5.8521 | 6.1880 | 6.6145 | 7.1834 | 8.0185 |
| VAPOR BOILUP-TO-FEED RATIO $\frac{V_S}{F}$ TRAY-TO-TRAY | 3.997 | 4.193 | 4.442 | 4.774 | 5.261 |
| % ENERGY INCREASE TRAY-TO-TRAY | 0 | 4.93 | 11.13 | 19.44 | 31.62 |
| REFLUX RATIO $R = \frac{L_R}{D}$ DOUGLAS-SEEMANN ANALYTICAL METHOD | 5.87 | 5.98 | 6.12 | 6.33 | 6.65 |
| % ENERGY INCREASE DOUGLAS-SEEMANN ANALYTICAL METHOD | 0 | 1.61 | 3.70 | 6.72 | 11.47 |

### REFERENCES