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Abstract

The set of Underwood equations developed for the sidestream stripper and the sidestream enricher easily extend to the Petlyuk configuration. Close scrutiny of these equations shows a family of middle component split fractions that give rise to minimum reflux. This insight facilitates a two part solution strategy. The analysis shown here is valid for any multicomponent feed mixture with any number of middle components.

Introduction

Petlyuk, et. al. (1965), described the configuration shown in Figure 1 as a feasible means to separate multicomponent mixtures. Until recently, a correct analysis of the Petlyuk configuration has required equilibrium stage calculations. It would be convenient to have a short-cut method that allows for quick evaluation of this configuration. Underwood's method (1946,1948), although initially developed for simple columns, can be extended to the Petlyuk configuration.

An understanding of non-sharp columns is critical to the analysis of the Petlyuk configuration. Underwood's method was initially extended to non-sharp columns by Shiras, et. al. (1950). In this analysis a linear system of Underwood equations is solved for the minimum vapor flow rate and the middle component split fractions. For the analysis of the Petlyuk column, however, it will be necessary to specify the distribution of some of the middle components. Therefore, a comprehensive form of Underwood's analysis applicable to the entire range of split fractions is necessary.

Fidkowski and Krolikowski (1986) develop a scheme to find the minimum vapor flow within the Petlyuk configuration. Their analysis is limited to ternary mixtures. The appropriate vapor flow rate is minimized subject to pinch point conditions and internal mass balances. The pinch conditions are expressed with Underwood's equations. An examination of the decision variables and the objective function shows the location of the optimal solution, and an analytical solution is found. The authors discover that minimum reflux occurs over a range of the middle component split fraction. Glinos and Malone (1988) also examine the Petlyuk column with a ternary feed mixture. Examination of the limiting flow conditions shows the existence of an infinite number of solutions. The authors then formulate several design rules as to when to favor various complex column configurations.

This paper will develop a generalized approach to the Petlyuk configuration analysis based on Underwood's original work. There will be no restriction placed on the number of middle components.

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First, Underwood's method for non-sharp columns will be extended to cover the entire range of middle component split fractions. A level of detail previously unexposed will be brought forth. The solution methods for side strippers and side enrichers are then applied to the Petlyuk configuration. From this understanding, regions of minimum reflux can be found. Since the analysis is often difficult, the development will be done in stages. One and two middle component cases will be shown in detail, and then generalizations will be made to the n middle component case.

Simple Non-Sharp Columns

In order to understand the Petlyuk configuration, a through understanding of simple non-sharp columns is necessary. A simple column has one feed (F) and two product streams, the distillate (D) and the bottoms (\pounds) . The components in the feed mixture are ranked in a list according to their volatility, and a light key and heavy key are designated for the column. Since the column is operated non-sharply, the key components will not be adjacent Components from the heavy key upward will appear in the distillate stream. The bottoms stream will contain components from the light key downward. Components that appear in both product streams are said to distribute. It will be convenient to divide the components into two sets. The components between the keys shall be designated the middle components (MC), and the remaining components shall be designated the non-middle components (NMQ. The split fraction for each component, \pounds_7 , is defined as the ratio of molar flow rates of the distillate stream to the feed stream. Thus, the split fraction can be expressed as

$$\xi_i = \frac{d_i}{f_i} \qquad (1 - \xi_i) = \frac{b_i}{f_i} \tag{1}$$

The split fraction represents the recovery of a component in the distillate stream. The Underwood equations for a simple column may be expressed in terms of split fractions as follows

$$\sum_{i} \frac{\alpha_{i} f_{i}}{\alpha_{i} - \phi_{j}} =$$

$$\sum_{i} \frac{\alpha_{i} \xi_{i} f_{i}}{\alpha_{i} - \phi_{j}} = D(R_{m} + 1) = V_{m}$$
(3)

$$\sum_{i} \frac{\alpha_{i} (1-\xi_{i}) f_{i}}{\alpha_{i}-\phi_{j}} = -S_{m} B = -\overline{V}_{m}$$
(4)

Here, *q* represents the quality of the feed. Underwood has shown that for *n* components between the keys there will be n + 1 roots, $\langle \mathbf{j} \rangle$, held in common between Equations 2, 3, and 4 such that

$$a_{LK} > \phi_1 > \alpha_{LK+1}$$

$$a_{LK} > \phi_1 > \alpha_{LK+1}$$

$$a_{LK-1} > a_{m-1} > a_{HK}$$

In all situations the composition and thermal condition of the feed will be given. In addition, specifications of some sort will be made on the product streams. For non-sharp columns it is typical to set the split fractions of the non-distributing components. Since components lighter than the light key will appear only in the distillate, their split fractions are set to 1.00. Likewise, the split fractions for components heavier than the heavy key are set to 0.00. Additionally, bounds are placed on the split fractions of the key components. That is, the recovery of the light key may be no worse than some lower bound and the split fraction of the heavy key may be no better than some upper bound

$$\xi_{LK} \geq \xi_{LK}^{LB} \qquad \xi_{HK} \leq \xi_{HK}^{UB} \tag{5}$$

All non-sharp split calculations have two degrees of freedom. If there are *n* middle components, Equation 3 can be written for each of the n + 1 roots. The light key and the heavy key plus the *n* middle components will distribute between the two product streams. Each of the distributing component split fractions is an unknown. The minimum vapor flow rate, V_m , is also an unknown. For *n* middle components there will be n + 1 equations and rt + 3 unknowns. Thus, there will be exactly two degrees of freedom for any number of middle components. In all situations the split fractions for two distributing components will be specified and the remaining split fractions and the minimum vapor flow rate will be calculated.

Shiras, et. al. (1950), extend Underwood's method and find the absolute minimum reflux for simple columns with n middle components. Initially, all of the relevant Underwood roots are found with Equation 2. These roots depend only on the feed composition and relative volatility, and therefore they will be constant. Next, Equation 3 is written for each root. To find the absolute minimum reflux, the split fractions of the key components are specified at their bounds. The middle component split fractions and the vapor rate are the unknowns. This is a linear system of equations of the form

$$\begin{bmatrix} a_{1}(\phi_{1}) & \cdots & a_{n}(\phi_{1}) & 1 \\ a_{1}(\phi_{2}) & \cdots & a_{n}(\phi_{2}) & 1 \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots \\ a_{1}(\phi_{n}) & \cdots & a_{n}(\phi_{n}) & 1 \\ a_{1}(\phi_{n+1}) & \cdots & a_{n}(\phi_{n+1}) & 1 \end{bmatrix} \begin{bmatrix} \xi_{1} \\ \xi_{2} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ \xi_{n} \\ V_{m} \end{bmatrix} = \begin{bmatrix} b_{NMC}(\phi_{1}) \\ b_{NMC}(\phi_{2}) \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ b_{NMC}(\phi_{n}) \\ b_{NMC}(\phi_{n+1}) \end{bmatrix}$$

where

$$a_{k}(\phi_{j}) = -\frac{\alpha^{*j^{*}}}{\alpha_{k} - \phi_{j}}$$
$$b_{NMC}(\phi_{j}) = \sum_{i \in NMC} \frac{\alpha_{i} \xi_{i} f_{i}}{\alpha_{i} - \phi_{j}}$$

The solution of this system yields the smallest minimum reflux possible for the column and the split fractions at which it will occur. Solutions for the Petlyuk configuration, however, will require split fractions other than the values associated with the absolute minimum solution. It is necessary, therefore, to be able to analyze non-sharp columns over the entire range of middle component split fractions.

Consider the case where there is one middle component There will be two relevant roots found from Equation 2 such that $a_{LK} > \$i > o_{MC} > \sphericalangle_2 > a_{HK}$. For this case there will be two specified split fractions and two unknowns. The goal is to be able to calculate the minimum vapor rate, V_{m} , over the entire range of the middle component split fraction \pounds_{MC} . The absolute minimum vapor rate is found by solving the following linear system

$$\begin{bmatrix} -\frac{\alpha_{MC}f_{MC}}{{}^{a}_{MC} - \phi_{1}} & 1 \\ -\frac{\alpha_{MC}f_{MC}}{{}^{a}_{MC} - \phi_{2}} & 1 \end{bmatrix} \begin{bmatrix} \xi_{MC} \\ V \\ m \end{bmatrix} = \begin{bmatrix} \sum_{i \neq MC} \frac{\alpha_{i} \xi_{i}f_{i}}{\alpha_{i} - \phi_{1}} \\ \sum_{i \neq MC} \frac{\alpha_{i} \xi_{i}f_{i}}{\alpha_{i} - \phi_{2}} \end{bmatrix}$$
(7)

In this system the light key is split from the heavy key with the middle component distributing. Thus, the

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(6)

key component split fractions are specified to be their bounds and the middle component split fraction is calculated. Let \pounds^{c} be the middle component split fraction that corresponds to the absolute minimum solution. At this point both Underwood roots are considered active.

Suppose $|_{MC}$ is specified at some value and that this value is less than $^{\circ}_{c}*$. Since there are two degrees of freedom an additional specification must be made. It is logical to specify the light key split fraction, %UP to be its lower bound. Thus, the heavy key split fraction, $%_{HK}$, and the minimum vapor rate are the calculated variables. This set of specifications yields the following linear system

$$\begin{bmatrix} -\frac{\alpha_{HK}}{\alpha_{HK} - \phi_1} & 1 \\ -\frac{\alpha_{HK}f_{HK}}{\alpha_{HK} - \phi_2} & 1 \end{bmatrix} \begin{bmatrix} \xi_{>HK} \\ V_m \end{bmatrix} = \begin{bmatrix} -\frac{\alpha_i \xi_i f_i}{ihiK^{*i-<\phi_1}} \\ y_m \\ iHK^{-\frac{\alpha_i \xi_i f_i}{a_i - *2}} \end{bmatrix}$$
(8)

As the middle component split fraction moves away from $%_{MC}^*$ and gets smaller, the heavy key split fraction will decrease from its upper bound. Thus, the calculated values of $%_{HK}$ will always remain within its bounds. At some transition point, Z_{HK} will equal 0.00. Solutions to this system with $^{\Lambda}_{MC}$ less than this transition value will give $%_{HK}$ less than 0.00. For middle component split fractions less than this transition point, the heavy key will no longer appear in the distillate stream. It is at this point that ϕ_2 becomes inactive and ($^$ remains as the only active root For middle component split fractions less than this transition value only a single Underwood equation is needed. The minimum vapor flow rate may be found by solving Equation 3 with ϕ_j as the root.

Suppose that \mathscr{H}_{MC} is specified at some value greater than $\pounds \mathcal{H}_{C}$. The heavy key, \wedge_{HK} , is then specified at its upper bound. This leads to the following linear system

$$\begin{bmatrix} -\frac{\alpha_{LK}f_{LK}}{\alpha_{LK}-\phi_{1}} & 1 \\ -\frac{\alpha_{LK}f_{LK}}{\alpha_{LK}-\phi_{2}} & 1 \end{bmatrix} \begin{bmatrix} \xi_{LK} \\ V_{m} \end{bmatrix} = \begin{bmatrix} \sum_{\substack{i \neq LK}} \frac{\alpha_{i}\xi_{i}f_{i}}{\alpha_{i}-\phi_{1}} \\ \vdots \neq LK \end{bmatrix} (9)$$

In this case the light key split fraction and the minimum vapor rate are the calculated variables. As the middle component split fraction moves away from $%_{MC}$ * and gets larger, the light key split fraction increases from it lower bound. Again, the calculated values of \backslash_{LK} will always remain within its bounds.

At some transition point $^{\circ}$ will equal 1.00. At middle component split fractions larger than this transition value, there will be no light key appearing in the bottoms stream. It is at this transition point that $^{\circ}$ becomes inactive. For middle component split fractions larger than this transition point the minimum vapor flow rate may be found by solving Equation 3 with \Rightarrow_2 as the root.

Calculation of the transition points is straightforward. The point where the heavy key no longer appears in the distillate stream may be found by solving Equation 7 with $%_{HK}$ set to 0.00. Likewise, The middle component split fraction at which the light key no longer appears in the bottoms stream can be found by solving Equation 7 with $t_{,LK}$ set to 1.00. This method also yields the vapor flow rate at the transition points.

For the one middle component case there will be four regions of middle component split fraction each characterized by a different set of specifications and active Underwood roots. Table 1 summarizes each region. The minimum vapor flow rate is a linear function of the middle component split fraction. A typical plot of these lines is shown in Figure 3. In this figure the minimum vapor flow rate is plotted against the middle component split fraction. The dashed vertical lines mark the transition points. The solid lines represent the appropriate function for each region. The slopes for regions I and II will always be negative while slopes for regions III and IV will always be positive. As the absolute minimum is approached the slopes get steeper. Regions II and III are typically very narrow. Their width is dependent on the bounds for the key component split fractions. When the bound for $\pounds >_{LK}$ is set at 1.00 and \wedge_{HK} is set at 0.00, all four lines will intersect at the same point. For this situation the four regions degenerate into two. As the separation becomes less difficult regions II and III become larger.

The linear relationships between the vapor flow rate and the middle component split fraction can be easily found. Using the information from the calculation of the transitions points, plus the vapor flow rate associated with $%_{MC} = 0.00$ and $%_{MC} = 1.00$, the appropriate slope and intercept can be determined for each region. It is also possible to derive analytic expressions for each region. These derivations are given in Appendix A.

Consider the case where there are two middle components. Equation 2 gives three roots such that ${}^{a}LK > {}^{1} > {}^{a}MC > {}^{5}2 > {}^{a}MC2 > {}^{3}3 > {}^{a}HK$. For s case ${}^{t}{}^{hiere} = {}^{w}{}^{hiere} = {}^{w}{}^{hiere} = {}^{t}{}^{hiere} = {}^{t}{}^{hi$

bounds. For regions I, II, and III the light key and first middle component split fractions, ξ_{LK} and ξ_{MC1} , are specified. Moving away from the absolute minimum solution toward smaller middle component split fractions two transition points are encountered. Initially in region III all three roots are active and ξ_{MC2} , ξ_{HK} , and V_m are the unknowns. The following linear system must be solved

$$\begin{bmatrix} -\frac{\alpha_{MC2}f_{MC2}}{\alpha_{MC2}-\phi_1} & -\frac{\alpha_{HK}f_{HK}}{\alpha_{HK}-\phi_1} & 1 \\ -\frac{\alpha_{MC2}f_{MC2}}{\alpha_{MC2}-\phi_2} & -\frac{\alpha_{HK}f_{HK}}{\alpha_{HK}-\phi_2} & 1 \\ -\frac{\alpha_{MC2}f_{MC2}}{\alpha_{MC2}-\phi_3} & -\frac{\alpha_{HK}f_{HK}}{\alpha_{HK}-\phi_3} & 1 \end{bmatrix} \begin{bmatrix} \xi_{MC2} \\ \xi_{HK} \\ \xi_{HK} \\ \xi_{HK} \end{bmatrix} = \begin{bmatrix} \sum_{\substack{i \neq MC2,HK}} \frac{\alpha_i \xi_i f_i}{\alpha_i - \phi_2} \\ \sum_{\substack{i \neq MC2,HK}} \frac{\alpha_i \xi_i f_i}{\alpha_i - \phi_2} \\ \sum_{\substack{i \neq MC2,HK}} \frac{\alpha_i \xi_i f_i}{\alpha_i - \phi_3} \end{bmatrix}$$
(10)

At the first transition point ξ_{HK} will equal 0.00 and ϕ_3 becomes inactive. From this point onward the heavy key will not appear in the distillate. In region II the unknown variables are ξ_{MC2} and V_m ; the appropriate system to solve is similar to Equation 8. At the second transition point ξ_{MC2} will equal 0.00 and ϕ_2 becomes inactive. From this point onward the second middle component will no longer appear in the distillate. In region I the only unknown variable is V_m . The minimum vapor flow rate may be calculated from Equation 3 with ϕ_1 as the root. In regions IV, V, and VI the second middle component and the heavy key split fractions, ξ_{MC2} and ξ_{HK} , are the specified variables. Again, two transition points are encountered moving away from the absolute minimum solution toward larger middle component split fractions, the first with $\xi_{LK} = 1.00$ and the second with $\xi_{MC1} = 1.00$. Regions IV through VI have three, two and one active roots respectively.

For each of the six regions a linear relationship exists that relates the minimum vapor flow rate to the appropriate middle component split fraction. For regions I, II, and III the minimum vapor flow rate is dependent on ξ_{MC1} while in regions IV, V, and VI the minimum vapor flow rate is dependent on ξ_{MC2} . Cramer's rule can be used to obtain analytical expressions from the appropriate linear system. Figure 4 shows a typical plot of minimum vapor flow rate against middle component split fraction. Note the change of scale on the abscissa. For regions I, II, and III the minimum vapor flow rate is plotted against the first middle component (the specified variable) while in regions IV, V, and VI it is plotted against the second middle component. The appropriate relationship for each region is shown with a solid line. As before, the regions adjacent to the minimum (III and IV) tend to be narrow and the slopes of these lines get steeper as the minimum is approached.

Linear relationships may also be derived between the specified and calculated middle component split fractions for regions II, III, IV, and V. The six regions may also be represented on a plot of $%_{MCI}$ versus ξ_{MC1} as shown in Figure 5. Here the solid line represents the appropriate relationship between \backslash_{MCI} and ξ_{MC2} region.

The previous cases may be generalized for n middle components. For the absolute minimum solution the bounds are specified for the key component split fractions. All of the roots will be active. For middle component split fractions less than the absolute minimum solution there will be n regions. The light key and first middle component split fractions will be specified in all of these regions. In the region adjacent to the absolute minimum solution, all of the roots will be active. Moving away from the minimum each successive region will have one less active root. There will be another n regions for middle component and heavy key split fractions are specified. The specification scheme for n middle components is summarized in Table 3.

The ability to formulate and solve simple non-sharp columns is now complete. Since the prefractionator of the Petlyuk configuration essentially acts as a non-sharp column, this knowledge is necessary for the following analysis.

Petlyuk Configuration

The Petlyuk configuration (Figure 1) consists of a prefractionator and a secondary column with a liquid sidestream. A pair of intermediate liquid and vapor streams pass from the prefractionator to the secondary columa. The system has one feed and three product streams which are designated P_{ν} , P_{2} , and P_{3} . The feed composition and quality are given. Specifications are made on the composition of the three product streams; the compositions of the intermediate streams are unknown. It is assumed that the overall goal of the system is to separate the feed into three product streams.

Typically, a light key and a heavy key are designated for the whole system. The light key and lighter components will appear in stream P_{ν} while the heavy key and heavier components will appear in stream P_3 . The middle components will appear in stream P_2 . To accomplish such a separation the prefractionator must split non-sharply with the middle components distributing.

The Petlyuk configuration is quite complex. The first step in the analysis is to transform the configuration into something that is easier to handle. To accomplish this goal the secondary column is divided into two

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separate columns at the sidestream tray. The new configuration is shown in Figure 2. A side stripper and side enricher are used in conjunction with the prefractionator. The bottom stream of the side stripper and the distillate stream of the side enricher together form the liquid sidestream product. Thus, the Petlyuk configuration can be thought of as the aggregate of a sidestream stripper and a sidestream enricher.

From the understanding of side strippers and side enrichers, the Underwood equations for the Petlyuk configuration may be written directly (Carlberg and Westerberg, 1988a). The prefractionator is analogous to a simple non-sharp column with the net product streams Dj and f?j. Thus, the Underwood equations for the prefractionator are

$$\sum_{i} \frac{\alpha_{i} J_{i}}{\alpha_{i} - \phi} = F(1 - q_{1})$$
⁽¹¹⁾

$$\sum_{i} \frac{\alpha_{i} d_{1i}}{\alpha_{i} - \phi} = D_{1} (R_{1m} + 1) = V_{1m}$$
(12)

$$\sum_{i} \frac{\alpha_{i} b_{1i}}{\alpha_{i} - \phi} = -S_{1m} B_{1} = -\overline{V}_{1m}$$
(13)

The prefractionator splits the feed according to the key components with the middle components distributing between the product streams.

The side stripper is analogous to a simple sharp column with a supertieated feed. Its Underwood equations are

$$\sum_{i} \frac{\alpha_{i} d}{\alpha_{i} -} = D_{1} (R_{1} + 1) = V_{1}$$
(14)

$$\sum_{i} \frac{\alpha_{i} d_{2i}}{\alpha_{i} - \eta} = D_{2} (R_{2m} + 1) = V_{2m}$$
(15)

$$\sum_{i} \frac{\alpha_{i} b_{2i}}{\alpha_{i} - \eta} = -S_{2m} B_{2} = -\overline{V}_{2m}$$
(16)

The Underwood root for the side stripper is denoted by TI. The side stripper splits its feed sharply between the light key and the next heaviest component.

The side enricher is analogous to a simple sharp column with a subcooled feed. The Underwood equations are

$$\sum_{i} \frac{\alpha_{i} b_{1i}}{\alpha_{i} - \Psi} = -S_{1} B_{1} = -\overline{V}_{1}$$
(17)

$$\sum_{i} \frac{\alpha_{i} d_{3i}}{\alpha_{i} - \psi} = D_{3} (R_{3m} + 1) = V_{3m}$$
(18)

$$\sum_{i} \frac{a_{i} \ b_{3i}}{\alpha_{i} - \psi} = -S_{3m} B_{3} = -\overline{V}_{3m}$$
(19)

Here, \|/ represents the Underwood root for the side enricher. The side enricher splits its feed sharply between the heavy key and the next lightest component.

The individual column outputs are related to the feed and product streams as follows

$$d_{1i} = \zeta_i f_i$$

$$b_{1i} = (1 - \zeta_i) f_i$$

$$< hi = Pu$$

$$^b li = \% i f_i \sim Pu$$

$$d_{3i} = (1 - \zeta_i) f_i - p_{3i}$$

$$^b 3i = P 3i$$

(20)

An examination of these relationships reveals that at least as much light key must appear in D_x as there is specified to appear in D_2 . Likewise, as least as much heavy key must appear in B^{\wedge} as there is specified to appear in By These requirements set the bounds for the key component split fractions in the prefractionator.

In addition to the Underwood equations, there is one constraint imposed on the representation. The mass balance at the liquid sidestream tray must be satisfied. Specifically,

$$\overline{V}_2 = V_3$$
 or $\overline{L}_2 = P_2 + L_3$ (21)

Since the internal vapor flow rates are represented by the Underwood equations, it is more convenient to use the vapor flow rate mass balance. By adjusting the split fractions of the middle components in the prefractionator, the internal flows of the side stripper and side enricher can be controlled. The general scheme of the analysis will be to find middle component split fractions that give rise to vapor flow rates that satisfy the mass balance. Equations 11 through 19 can be handled by using the techniques for non-sharp columns and side strippers and side enrichers. Before a solution method can be given, however, more insight must be gained by a closer examination of the equations.

Consider the situation where there is only one middle component As the middle component split fraction increases the feed to the side stripper increases and the feed to the side enricher decreases. As a consequence, the vapor flow rate at the bottom of the side stripper, \overline{V}_2 , ${}^{m\,u\,s\,t}$ increase and the vapor flow rate at the bottom of the side stripper, \overline{V}_2 , ${}^{m\,u\,s\,t}$ increase and the vapor flow rate at the top of the side enricher, V_3 , must decrease. Since \overline{V}_2 and V_3 form the mass balance constraint, it will be convenient to designate these internal flows as the mass balance flow rates. A typical plot of the mass balance flow rates is shown in Figure 6. Note that the slopes of the mass balance flow rates change from one region to the next. There will only be one value for the middle component split fraction, $|_{MC}|$ that will satisfy the mass balance at the side stream tray. The mass balance point can occur in any region; in Figure 6 the mass balance point is in region I.

The side stripper root will be found in the range $a_{LK} > r_1^{f} > a_{MC}$. This is the same interval as the prefractionator root \S_l for column 1. A close examination of Equations 12 and 14 reveals that these equations must be the same when ()₁ is active. Hence, in regions I, II, and III, the root r| will be constant and identical to $^{\wedge}$ Since the product specifications are fixed, the vapor rate V_2 will be constant over the same regions. V_2 will be an increasing function with respect to middle component split fraction in region IV. A similar situation occurs between Equations 17 and 13. The side enricher root y and the prefractionator root \diamondsuit_2 occur over the same range. When \diamondsuit_2 is active, the two equations are the same. Thus, in regions II, III, and IV, the root y will be constant and identical to \bigstar_2 As a result the vapor rate \overline{V}_3 will be constant in the same regions. \overline{V}_3 will be a decreasing of $^{\wedge}_{MC}$ function in region I. The vapor flow rate at the top of the side stripper, V_2 , and the vapor flow rate at the bottom of the side enricher, \overline{V}_3 , are proportional to the utility consumption of the Petlyuk column. For convenience, these parameters will be designated as the utility flow rates.

The mass balance flow rates and the utility flow rates are related as follows. The vapor mass balance at the feed tray in the side stripper

$$V_x + \vec{V}_2 = V_2 \tag{22}$$

and the vapor mass balance at the feed tray in the side enricher

$$\overline{V}_3 = \overline{V}_l + V_3 \tag{23}$$

may be added together to obtain

$$V_1 + \overline{V}_2 + \overline{V}_3 = \overline{V}_x + V_2 + V_3$$
 (24)

Noting that $V_x - \overline{V}^{\wedge}$ is equal to F (1 - q), this equation can be expressed as

$$F(l-q) + V_2 + 7_3 = V_2 + V_3$$
(25)

When the mass balance at the sidestream tray is satisfied, the utility vapor flows are related as follows

$$F(l-q) + V_3 = V_2$$
 (26)

As a special case, when the feed is a saturated liquid (q = 1), V_2 will equal \overline{V}_3 at the mass balance point. A typical plot of the utility vapor flow rates is shown in Figure 7.

The mass balance at the sidestream tray must always hold. If the prefractionator is not operated at \mathscr{H}_{MC} the mass balance may still be satisfied by increasing the reflux or reboil of the side columns as necessary. If \overline{V}_2 is less than V_{3S} then additional reflux is required in the side stripper to satisfy the mass balance. Conversely, more reboil is required in the side enricher if \overline{V}_2 is greater than V_3 . Figure 8 shows the feasible mass balance flow rates when the mass balance falls in region I. This set of mass balance flow rates gives rise to the corresponding utility flow rates shown in Figure 9. A region, rather than a point, of minimum reflux is present due to the constant portions of the utility flow rates.

The region of minimum reflux may be stated explicitly for the single middle component case. If the mass balance point, % MQ is less than the absolute minimum split fraction, C1* , then minimum reflux will occur from the mass balance point to the transition point between region III and IV. If the mass balance point is greater than the absolute minimum split fraction, then minimum reflux will occur from the transition point between region I and II to the mass balance point. In all cases the split fraction corresponding to the absolute minimum solution will be in the region of minimum reflux. These insights allow the formulation of a two part solution strategy.

In the first portion, the minimum vapor flow rates for the configuration are found by using the split fraction associated with the absolute minimum solution for the prefractionator. Initially, Equation 11 is solved for \triangleleft_1 and \triangleleft_2 Equation 7 is then set up and solved for $\$_{MC}^*$ and V_{ν} With this split fraction known the net output streams of the prefractionator are set. \overline{V}_l can be determined with Equation 13 with either of

the roots. The Underwood roots for the side columns are found next. Equation 14 is solved for r| and Equation 17 is solved for y. With the side column roots known the utility vapor flow rates, V_2 and $\vec{\nabla}_3$, are calculated with Equations 15 and 19 respectively. The larger of these two values will be the overall minimum vapor rate for the Petlyuk configuration.

In the second part of the solution strategy the extent of the minimum reflux region is determined. The middle component split fraction is adjusted until the mass balance point, $\% MC^*$ is found. Before this step may begin a full characterization of the non-sharp regions in the prefractionator is necessary. Initially a split fraction is guessed. Depending upon which region the guess may fall into, the appropriate equation is used to determine the prefractionator vapor flow rate. The Underwood roots for the side columns are determined and the mass balance flow rates, \overline{V}_2 and V_3 , are calculated with Equations 16 and 18. If the mass balance is not satisfied, the middle component split fraction is adjusted and the procedure is repeated.

The situation for two middle components is similar. For this case there will be three Underwood roots and six non-sharp regions for the prefractionator. According to the specification scheme, the first middle component split fraction will be the degree of freedom for regions I, II, and III. For regions IV, V, and VI the second middle component split fraction will be specified. As before, \overline{V}_2 will increase and V_3 will decrease as the middle component split fractions increase. As shown in Figure 10 there will be one point that satisfies the mass balance. The corresponding utility flow rates are shown in Figure 11. V_2 will be constant in the regions where $^{\circ}$ is active. This occurs in regions I, II, III, and IV. In regions III, IV, V, and VI, where \Rightarrow_3 is active, \overline{V}_3 is constant. The constant portions of the utility flow rates give rise to a region of minimum reflux. The set of middle component split fractions corresponding to this region can be seen on a plot of $^{\circ}C 2^{versus} \pounds A/C1 \land Figure 12$.

From these two cases the solution procedure may be generalized for *n* middle components. In this case the prefractionator will have AI+ 1 roots and 2n non-sharp regions. For split fractions below the absolute minimum solution the lightest middle component split fraction is the degree of freedom. For split fractions greater than the absolute minimum solution the heaviest middle component split fraction is the specified variable. A general solution scheme may be stated. First, find the absolute minimum solution for the prefractionator. Use the split fractions found in this calculation to find the remaining component flow rates in the configuration. Find the roots for the side columns and calculate the utility flow rates. Take the largest value as the overall minimum vapor flow rate for the configuration. Next, find the extent of the minimum reflux region; search over the range of split fractions for the mass balance point Guess either the lightest or heaviest middle component split fraction. Use the appropriate relationships, depending upon which region the specification is in, and calculate the remaining split fractions and the prefractionator flow rates. Find the side column roots and calculate the mass balance flow rates. If the mass balance is not satisfied, update the split fractions and calculate again. If the mass balance point is below the absolute minimum solution then the minimum reflux region will extend from the mass balance point to the transition point between region n+1 and n+2. If the mass balance point is above the absolute minimum solution then the minimum reflux region the transition point between region n-1and n and the mass balance point. Figure 13 summarizes the possible minimum reflux regions.

The following example demonstrates the solution procedure. A six component mixture is to be separated into three product streams. The feed and product specifications are given in Table 4. The feed is a saturated liquid, and the products are removed at their bubble points. The specifications show that the split fraction bound for component A, the light key, is .995; the bound for component D, the heavy key, is .005. The prefractionator has been characterized and the relationships that govern each of the non-sharp regions are summarized in Table 5. The absolute minimum solution occurs at $\%_B = .7446$ and $\uparrow_c = .0773$. This set of split fractions is used to solve the remaining equations for the utility flow rates. V_2 was calculated to be 397.0 kg-mol/hr and \overline{V}_3 was found to be 424.8 kg-mol/hr. Thus, the overall minimum vapor flow rate is the larger of the two values. The middle component split fractions are searched for the mass balance point. In this example the mass balance point occurs in region V at $Z_{3B} = .8556$ and $\pounds_c = .0836$. Since the mass balance point is greater than the absolute minimum point, the region of minimum reflux extends from the II-III transition point to the mass balance point. Thus, in this example, the minimum reflux occurs over the range from $\%_B = .7434$ and $\uparrow_B = .0728$ to $\uparrow_B = .8556$ and $\uparrow_= .0836$.

Utility Consumption

The Petlyuk configuration, like other complex column configurations, is more favorable with respect to first law effects and less favorable with respect to second law effects. That is, the Petlyuk configuration will consume less utilities but will have a larger temperature drop relative to other analogous configurations. Pictured in Figure 14 is (a) the Petlyuk configuration, (b) its simple column analog, and (c) a side stripper/enricher configuration. Each of these configurations will be examined for their first and second law tradeoffs. In order for all three configurations to be completely analogous, the first column of configurations (b) and (c) must perform a non-sharp split similar to the prefractionator of the Petlyuk configuration. The two side columns in (b) and (c) operate sharply. The same separation occurs in each

analogous column. In this discussion the condenser and reboiler duties for the analogous configurations will be denoted with an appropriate prime superscript as shown in Figure 14.

Terranova and Westerberg (1988) show that as the feed to a simple column becomes more superheated, the condenser duty must increase and the reboiler duty must decrease. Conversely, as the feed to a simple column becomes more subcooled, the reboiler duty must increase and the condenser duty must decrease. These insights can be used to show that the side stripper and the side enricher consume less utilities than the respective simple column analogs (Carlberg and Westerberg, 1988a). Since the Petlyuk configuration and its simple column analog are the aggregate of these cases, these relationships may be applied here. Specifically, the following relationships hold between the Petlyuk configuration and its simple column analog

$$Q_{C2} < Q_{C1}' + Q_{C2}' \tag{27}$$

$$Q_{R3} < Q_{R1}' + Q_{R3}'$$
 (28)

Although these relationships were derived for columns performing sharp separations, they hold for any set of middle component split fractions as long as they are the same for both configurations. The simple column analog has additional utility requirements on the bottoms stream of the second column and the distillate stream of the third column. In terms of the cold utility, the following holds directly from Equation 27

$$Q_{C2} < Q_{C1}' + Q_{C2}' + Q_{C3}'$$
 (29)

while from Equation 28 for the hot utility, the result is

$$Q_{R3} < Q_{R1}' + Q_{R2}' + Q_{R3}'$$
(30)

Thus, the Petlyuk configuration will consume less utilities, and hence be more favorable with respect to the first law, than the analogous simple column configuration.

In the Petlyuk configuration, vapor streams pass between the prefractionator and the secondary column. For this to occur there must be a slight difference in pressure between the point supplying vapor and the point receiving vapor. This will occur naturally in this configuration by virtue of the pressure drop from the reboiler to the condenser. Hence, both columns in the Petlyuk configuration must operate at the same nominal pressure. As a consequence, there will be a large temperature difference between the reboiler and condenser. Thus, despite the utility savings, the Petlyuk column is favorable only when there is a wide temperature range between the heat sources and sinks. Since the utilities must be at more extreme temperatures for the Petlyuk configuration, these utilities will be more costly. There is also likely to be a

smaller temperature driving force between the reboiler and condenser and the utilities. Hence, the Petlyuk configuration requires a sizable capital equipment investment for heat exchange area. A typical T-Q diagram for a Petlyuk configuration, along with a hot and cold utility, are shown in Figure 15.

For simple columns, liquid streams pass from one column to the next Pumps or valves can be used to change the pressure of each column. The pressure of each simple column is independent and may be set so as to minimize the difference between the hottest and coldest point in the configuration. Figure 16a shows a typical T-Q diagram for the simple column analog. The pressures for the simple columns were chosen to minimize the temperature difference across the configuration. Thus, simple columns are favored when there is a narrow range of temperature between the available heat sources and sinks. Heat may be supplied and removed to the simple columns at less extreme and more cost effective temperatures.

As a variation, the second and third column of the simple column analog may be heat integrated with the selection of appropriate pressures. In this scheme, the heat given off by the condenser of the third column is used to drive the reboiler of the second column. The T-Q diagram for this configuration is shown in Figure 16b. Because Q_{R} and QQ^{\wedge} are integrated, this configuration has the advantage of requiring less total utilities than the simple column analog of Figure 16a. Still, as Equations 27 and 28 indicate, this scheme will require more utilities than the Petlyuk configuration. As a disadvantage, the heat integrated simple column design requires a temperature range similar to the Petlyuk configuration.

As a further variation, a partial condenser may be used on the first column. The effect of the partial condenser will be to decrease the load on the condenser of the first column, \pounds_{C1} , and the reboiler of the second column, Q_{R2} . The condenser load of the second column, Qc > ^w increase. The remaining reboiler loads, Q_{Rl} and Q_{R3} do not change. Thus, the total utility requirements are smaller for this scheme than simple column designs with a total condenser. Figure 16c shows the T-Q diagram for this design. Since the heat into the first and second columns does not balance the heat out, these columns are no longer represented as rectangles on a T-Q diagram. Once again, there is a tradeoff between the total utility requirements and the temperature at which the utilities are supplied.

As a final consideration, the Petlyuk configuration should be compared to the side enricher/stripper configuration. In this scheme the reboiler of the side stripper may be heat integrated with the condenser of the side enricher. This requires a temperature difference between the two streams. Since both side columns are at the same nominal pressure, a suitable temperature difference will generally occur only when there are two or more middle components. Unlike the Petlyuk configuration, the side

stripper/enricher does not have a mass balance constraint. Hence, the configuration may be operated at any set of middle component split fractions that is desired. The information needed to compare these two cases is readily found in the mass balance and utility flow rate plots (Figures 6 and 7, for instance). For any set of middle component split fractions, the T-Q diagram for the side stripper/enricher is constructed with this information. Such a T-Q diagram, for the case where the middle component split fractions correspond to the absolute minimum solution, is shown in Figure 17.

Since the region of constant reflux represents the smallest vapor flow rates for the Petlyuk configuration, it is the area of interest for comparison of designs. Consider the case shown in Figures 6 and 7 where the set of split fractions that satisfy the mass balance is smaller than the set of absolute minimum split fractions. Examination of the utility vapor flow rates in Figure 7 shows

$$Qci = Qci^{\prime\prime}$$
 OD

$$QR3 > QR3'' \tag{32}$$

From Figure 6, the mass balance flow rates indicate

$$QRI'' > 2c3''$$
(33)

The difference between these two quantities,

$$QH = QRI'' \sim Qc3'' \tag{34}$$

is the heating requirement that must be made up with hot utilities. By an overall energy balance

$$Qci'' - Qta'' + QH$$
(35)

Thus, in light of Equation 31, the total utility consumption of the side stripper/enricher is the same as the Petlyuk configuration in the region of constant reflux. There is, however, an advantage to supplying a portion of the required heat, Q_H^* , at a lower temperature. For the case where the set of split fractions that satisfy the mass balance is larger than the set of absolute minimum split fractions, the reboiler load of the second column, Q_R is less than the condenser duty of the third column, Q_c . Th^e additional cooling requirement, Q_c^* , is made up with cold utilities. The advantage here is that the cooling may be supplied at a higher temperature.

In conclusion, these examples point out the tradeoffs between the first and second law. The Petlyuk configuration and the side stripper/enricher have a first law advantage in that they have low utility requirements. The Petlyuk configuration has a second law disadvantage because of the large temperature range of operation. The simple column designs have the opposite characteristics in larger utility consumption and a less extreme temperature range of operation.

Nomenclature

Variables

B	total molar flow rate of bottoms stream									
ty	molar flow rate of component i in bottoms stream									
D	total molar flow rate of distillate stream									
$d_{\dot{x}}$	molar flow rate of component / in distillate stream									
F	total molar flow rate of feed stream									
f_t	molar flow rate of component <i>i</i> in feed stream									
L	rectifying section liquid flow rate									
Ī	stripping section liquid flow rate									
P_k	total molar flow rate of product stream k									
Pto	molar flow rate of component / in product stream k									
Q_c	condenser heat duty									
Q_R	rebolier heat duty									
q	thermal quality of feed stream									
R	reflux ratio									
R_m	minimum reflux ratio									
S	reboil ratio									
$5_{\rm m}$	minimum reboil ratio									
T_c	condenser temperature									
T_R	reboiler temperature									
V	rectifying section vapor flow rate									
V_m	rectifying section minimum vapor flow rate									
\overline{V}	stripping section vapor flow rate									
\overline{V}_m	stripping section minimum vapor flow rate									
x_{Di}	mole fraction of component <i>i</i> in distillate stream									

x_{Bi}	mole fraction of component i in bottoms stream
a,∙	relative volatility of component i
<{>	primary column Underwood root;
£ _f .	split fraction of component <i>i</i>
^A/C*	middle component split fraction corresponding to absolute minimum solution
^> <i>MC</i>	middle component split fraction corresponding to mass mass balance point
r	side stripper Underwood root
У	side enricher Underwood root
a 1	
Subsci	ripts
HK	heavy key
LK	light key
МС	middle component one middle component case

MCI first middle component — two middle component case

MC2 second middle component -- two middle component case

MCn nth middle component

Appendix A

Linear relationships exist between the vapor flow rate and the middle component split fraction in all of the four nonsharp regions present in the one middle component case. Analytical expressions for these relationships may be derived as follows.

In region I $^$ is the only active root. Equation 3 written with this root is the appropriate relationship. To show the linearity the middle component term may be pulled out of the summation. Thus, the linear relationship is given by

$$V = \frac{\alpha_{Mcff4}C}{mc} \mathcal{I}_{ur} + \mathcal{I}_{ur}$$
(30)

In region II the situation is a bit different. For this region both roots are active and the heavy key split fraction, $|_{HK_J}$ is an unknown. Thus, an expression for the heavy key split fraction as a function of the

middle key split fraction is needed. To obtain this expression Equation 3 is written twice, once for each root. The left hand sides of these expressions are equated, and after some algebra the following result is obtained

$$\xi_{HK} = -\frac{(\alpha_{HK} - \phi_1)(\alpha_{HK} - \phi_2)}{\alpha_{HK}f_{HK}} \sum_{i \neq HK} \frac{**\% ft}{(\alpha - \phi_1)(\alpha_i - \phi_2)}$$
(37)

Equation 37 may be substituted into Equation 3 for either root. When ^ is used in Equation 3 the linear result is

$$V = \frac{\alpha_{MC}f_{MC}}{\alpha_{MC} - \phi_1} \left(1 - \frac{a_{HK} + \phi_2}{\alpha_{MC} - \phi_2}\right) \xi_{MC} + \sum_{\substack{i \neq MC, HK}} \frac{\alpha_i \xi_i f_i}{\alpha_i - \phi_1} - (\alpha_{HK} - \phi_2) \sum_{\substack{i \neq MC, HK}} \frac{\alpha_i \xi_i f_i}{(\alpha_i - \phi_1) (\alpha_i - \phi_2)}$$
(38)

The derivation for region III is similar to region II. Here $|_{LK}$ is unknown. The light key split fraction is related to the middle component split fraction by

$$\xi_{LK} = -\frac{(\alpha_{LK} - \phi_1)(\alpha_{LK} - \phi_2)}{\alpha_{LK}f_{LK}} \sum_{i \neq HK} \frac{\alpha_i \xi_i f_i}{(\alpha - \phi_1)(\alpha_i - \phi_2)}$$
(39)

Substituting Equation 39 into Equation 3 written with 4, the linear result is

$$V = \frac{\alpha_{MC} f_{MC}}{\alpha_{MC} - \phi_2} \left(1 - \frac{\alpha_i \xi_i f_i}{\alpha_i - \phi_2} - (\alpha_{HK} - \phi_1) \sum_{i \neq LK,MC} \frac{\alpha_i \xi_i f_i}{(\alpha_i - \phi_1) (\alpha_i - \phi_2)} \right)$$
(40)

Region IV is similar to region I although $< b_2$ is the active root. Equation 3 written with this root can be rearranged to obtain

$$V = \frac{\alpha_{MC} f_{MC}}{\alpha_{MC} - \phi_2} \xi_{MC} + \sum_{i \neq MC} \frac{\alpha_i \xi_i f_i}{\alpha_i - \phi_2}$$
(41)

Similar linear expressions may be found for cases with more than one middle component.

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region (point)	ξ <i>ικ</i>	Ę _{MC}	^к >нк	V _m	active <i>roots</i>
I	LB	DF	0.00	CALC	•1
Ш	LB	DF	CALC	CALC	\$ ₁ ,\$ ₂
(min)	LB	CALC	UB	CALC	\$1,\$2
ш	CALC	DF	UB	CALC	φ ₁ ,φ ₂
IV	1.00	DF	UB	CALC	\$ ₂

Table 1: One Middle Component Regions

LB = lower bound UB = upper bound

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DF = degree of freedom

CALC = calculated variable

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region (point)	ξικ	ξ <i>мC</i> 1	ξ _М С2	ξ <i>нк</i>	V _m	active roots
I	LB	DF	0.00	0.00	CALC	Φ ₁
II	LB	DF	CALC	0.00	CALC	φ ₁ ,φ ₂
III	LB	DF	CALC	CALC	CALC	φ ₁ ,φ ₂ ,φ ₃
(min)	LB	CALC	CALC	UB	CALC	φ ₁ ,φ ₂ ,φ ₃
IV	CALC	CALC	DF	UB	CALC	φ ₁ ,φ ₂ ,φ ₃
v	1.00	CALC	DF	UB	CALC	φ ₂ ,φ ₃
VI	1.00	1.00	DF	UB	CALC	ф 3

Table 2: Two Middle Component Regions

LB = lower bound

UB = upper bound

DF = degree of freedom

CALC = calculated variable

region	ξ _{<i>LK</i>}	ξ _{MC1}	ξ _{MCn}	₹ -> <i>HK</i>	V _m	active roots
(point)						
I	LB	DF	0.00	0.00	CALC	φ ₁
	•		•	•	•	,
	•			•	•	•
	•	•	•	•	•	•
<i>n</i> -\	LB	DF	CALC	0.00	CALC	$\phi_1 \cdots \phi_n$
n	LB	DF	CALC	CALC	CALC	•1 ••• <j>n+1</j>
(min)	LB	CALC	CALC	UB	CALC	$\phi_1 \cdots \phi_{n+1}$
n+1	CALC	CALC	DF	UB	CALC	$\phi_1 \cdots \ll_{n+1}$
n+2	1.00	CALC	DF	UB	CALC	$\phi_2 \cdots \phi_{n+1}$
		•				
					•	
2n	1.00	1.00	DF	UB	CALC	ф _{п+1}

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Table 3:	n Middle	Component	Regions
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LB = lower bound

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UB = upper bound

DF = degree of freedom

CALC = calculated variable

	component	a;	f_i	Pu	Pli	<i>p</i> _{3i}
A	ethanol	2.289	30.0	29.85	0.15	0.00
B	i-propanol	1.958	30.0	0.15	29.85	0.00
С	n-propanol	1.089	15.0	0.00	14.925	0.075
D	2-butanol	1.000	15.0	0.00	0.075	14.925
E	i-butanol	0.712	5.0	0.00	0.00	5.00
F	n-butanol	0.476	5.0	0.00	0.00	5.00

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Table 4: Example Problem -- Feed and Product Specifications

all flow rates in kg-mol/hr

Table 5: Example Problem -- Characterization of Prefractionator

RegionsVapor RelationshipsSplit Fraction RelationshipsI.0000 <%_B < .7317
$$V_I = -367.7 \%_B + 399.0$$
 $^{A} = \%_D = .0000$ II.7317 <%_B < .1A2A
.0000 < $\$_c < .0728$ $V_I = -466.2\pounds_{fl} + 471.1$ $\pounds_c = 6.207\$_{fl} - 4.541$
 $\%_D = .0000$ III.7434 <%_B < .7446
.0728 <%_c < .0773 $V_I = -484.6\%_B + 484.7$ $^{A} = 3.8204_{fl} - 2.767$
 $\pounds_D = 4.167\pounds_{fl} - 3.097$ IV.7446 < $\$_{fl} < .0773$ $V_I = -1710.4^{A} - 8.4$ $^{A}_{fl} = 10.204^{A}_{c} - 0.045$
 $\%_A = 12.500^{A}_{c} + .0288$ V.7483 < $\%_B < 1.000$ $V_x = 1466.4^{A}_{c} + 10.6$ $\pounds_B = 18.149^{A}_{c} - 0.662$
 $\%_{fl} = 1.0000$ VI.0916 < $\%c < 1.000$ $^{A} = 309.3^{A} + 116.5$ $^{A}_{A} = ^{A}_{fl} = 1.000$

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Figure 2: Equivalent Petlyuk Configuration





Figure 4:. Minimum Vapor Flow Rate as a Function of Middle Component Split Fraction -- Two Middle Components



Figure 5: Corresponding Middle Component Split Fractions --Two Middle Component Case



Figure 6: Mass Balance Flow Rates -- One Middle Component Case



Figure 7: Utility Flow Rates -- One Middle Component Case



Figure 8: Feasible Mass Balance Flow Rates - One Middle Component Case



Figure 9: Minimum Reflux Region - One Middle Component Case

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Figure 10: Mass Balance Flow Rates - Two Middle Component Case



Figure 11: Utility Flow Rates - Two Middle Component Case



Figure 12: Minimum Reflux Region - Two Middle Component Case



Figure 13: Possible Minimum Reflux Regions -- (a) mass balance point below minimum solution, (b) mass balance point above minimum solution.

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Figure 14: (a) Petlyuk Column (b) Simple Column Analog (c) Side Stripper/Enricher

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Figure 15: T-Q Diagram for Petlyuk Configuration







Figure 17: T-Q Diagram for Side Stripper/Enricher

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