Minimum Energy Consumption in Multicomponent Distillation
Part II:
Three-product Petlyuk Arrangements

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Abstract

We show that the minimum energy requirement for separation of a multicomponent mixture in a three-product Petlyuk arrangement is equal to the minimum energy for most difficult of the two separations (top/middle- or middle/bottom product) in a conventional single column. In the V_{min}-diagram (part I) this is simply the highest peak. These results are based on an analytical solution for columns with infinite number of stages, assuming constant relative volatilities and constant molar flows. The previous analytical results for the Petlyuk column are extended to include non-sharp separations, multicomponent feeds, and any feed quality.

Keywords: Petlyuk column, minimum energy, multicomponent distillation, Fully thermally coupled columns, Underwood equations.

1   Introduction

In this paper, the minimum energy expressions for the three-product Petlyuk arrangement[1] shown in Figure 1 are generalized to handle any feed quality and nonsharp product splits. We also illustrate by examples that we can easily handle more than three feed components. We use the simplifying assumptions of constant pressure, constant relative volatility (α) and constant molar flows, and consider the limiting case with infinite number of stages.
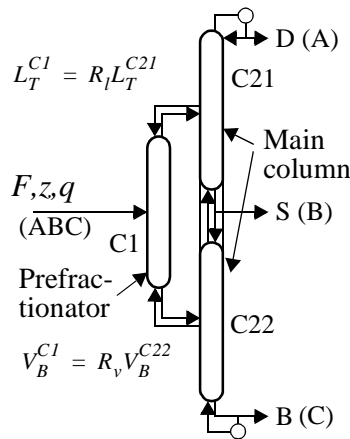

Figure 1: The integrated Petlyuk arrangement for separation of ternary mixtures.

The ternary feed (F) with components A (light), B (intermediate) and C (heavy) is supplied to the prefractionator (column C1), which performs the "easy" A/C split. The minimum vapour flow in the prefractionator column is obtained for a particular distribution of the intermediate B component, denoted as the *preferred split*[2]. This split also results in a minimum overall energy requirement in the Petlyuk column. Interestingly, this solution is not unique and several authors, e.g Fidkowski and Krolikowski[3] and Christiansen and Skogestad[4] have shown that the optimum can be obtained by operating the prefractionator in the whole region between the preferred split and the so-called "balanced" split where the vapour flow requirements in the bottom of column C21 and in the top of column C22 are equal. This implies that there is a "flat" optimality region and that the minimum vapour flow can be obtained not only at a single operating point, but along a line segment in the space spanned by the two degrees of freedom.

An analytical expression for the minimum vapour flow in a Petlyuk arrangement with a ternary feed and liquid sidestream was obtained independently by Fidkowski and Krolikowski[3] and Glinos et. al.[5] for the case of saturated liquid feed ($q=1$), and sharp product splits:

$$V_{min}^{Petlyuk} = max\left(\frac{\alpha_A z_A}{\alpha_A - \theta_A}, \frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{\alpha_B z_B}{\alpha_B - \theta_B} \right) F \qquad (1)$$

Here, θ_A, θ_B are the two common Underwood roots, obtained from equation (3) for the prefractionator feed.

Fidkowski and Krolikowski[3] derived equation (1) by a quite detailed algebraic procedure, via expressions for pinch-zone compositions at the connection points as functions of the operating point of the prefractionator. Here we will use another approach, more directly based on the Underwood equations. Such an approach was first presented by Carlberg and Westerberg[6,7], who also extended the solution to more than one intermediate component.

An important finding in our work is that the minimum energy requirement ($V_{min}^{Petlyuk}$) and the detailed vapour flow requirements may be obtained by just a glance at the V_{min}-diagram for a single two-product column. This was presented in Part I[8,9], and is computed based on Underwood's equations[10,11,12,13] for multicomponent distillation in conventional columns. The most important results from Part I are reviewed in Section 2.

In the directly coupled sections of the Petlyuk arrangement we have recycle flows from the main column into the top and the bottom of the prefractionator. This is a new situation compared to the conventional arrangements, and we must really check if Underwood's methods can be applied. This issue is treated in the thesis by Halvorsen[8], and it turns out that with some restrictions on the recycle stream compositions, the directly coupled columns can be treated as ordinary columns. In Section 3.2 we present the important result from Carlberg and Westerberg[6,7] on how the Underwood roots carry over to succeeding directly coupled column. This is the basis for the very simple assessment we can do with a V_{min}-diagram.

The main results for a ternary mixture are presented in Sections 4 and the results are generalized to more than three feed components and nonsharp product splits in Section 5.

In Section 6, we briefly discuss the results in relation to some other types of column integration.

2 Review of the Basic Equations for Minimum Energy

2.1 The Underwood Equations

Consider a two-product distillation column with a multicomponent feed (F) with liquid fraction q and composition vector z of N components. The defining equation for the Underwood roots (ϕ) in the top and (ψ) in the bottom are:

$$\text{Top: } V_T = \sum_{i=1}^{N} \frac{\alpha_i w_{i,T}}{\alpha_i - \phi} \quad \text{Bottom: } V_B = \sum_{i=1}^{N} \frac{\alpha_i w_{i,B}}{\alpha_i - \psi} \tag{2}$$

where w_i is the net flow of a component (defined positive upwards, also in the bottom). There will be N solutions for each root, and the solution sets from the top and bottom equations are generally different. However, Underwood[10,11,12,13] showed that the roots obey: $\alpha_i \geq \phi_i \geq \psi_{i+1} \geq \alpha_{i+1}$. Furthermore, with infinite number of stages, at minimum vapour flow, one or more pairs of roots (ϕ_i, ψ_{i+1}) in the top and bottom coincide to a set of common roots (θ_i). The set of (N-1) possible common roots are obtained by setting $\phi_i = \psi_{i+1} = \theta_i$ and subtracting the two defining equations above. This gives the feed equation where the set of common roots depends only on the feed properties α, z and q:

$$V_T - V_B = \sum_{i=1}^{N} \frac{\alpha_i(w_{i,T} - w_{i,B})}{\alpha_i - \theta} = \sum_{i=1}^{N} \frac{\alpha_i z_i F}{\alpha_i - \theta} = (1-q)F \tag{3}$$

However, it is not obvious when we may apply the common roots (θ) solved from (3) back into the defining equations (2), in particular for more than two components. The rule is that we may apply the common roots in the range of volatilities for the components distributed to both ends (including components exactly at the limit of

being distributed). We denote these *active roots*. When we have any active roots then: $V = V_{min}$. The minimum vapour flow and component distribution can then be found by solving the equation set obtained by applying all the *active* roots in (2). Two degrees of freedom (e.g. two key component recoveries) must be specified. If there are no active roots: $V > V_{min}$.

2.2 The V_{min}-diagram for a Single Conventional Column

We here review the results from Part I[8,9]. Since a two-product column operated at constant pressure has only two degrees of freedom we may visualize all possible operating points in the *D-V* plane. This is illustrated in the V_{min}-diagram, which is shown for a ternary feed (with components ABC) in Figure 2.
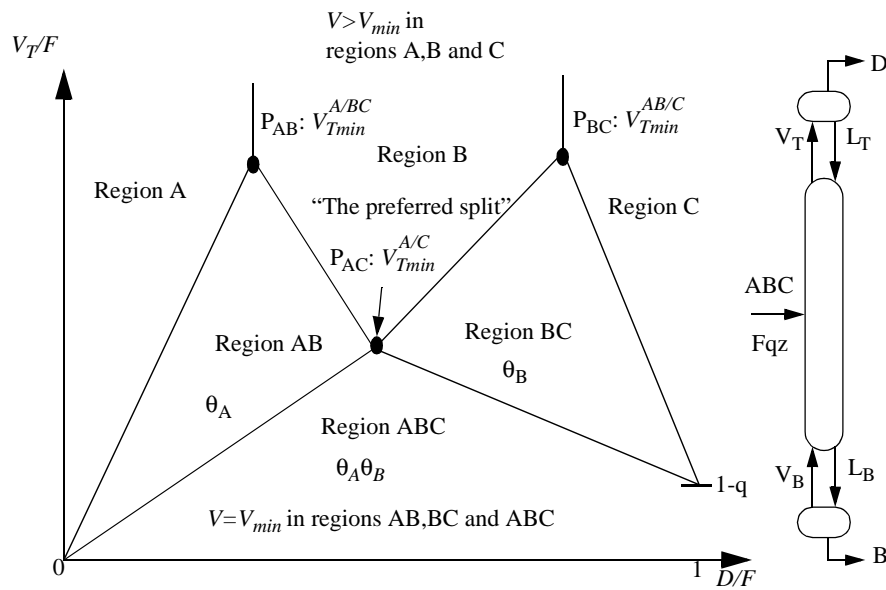

Figure 2: The V_{min}-diagram for a ternary mixture ABC. The components which are distributed to both ends are indicated in each region, with the corresponding active Underwood roots.

Each peak or knot in this diagram (P_{ij}) is the operating point for minimum vapour flow and sharp split between the component pair i,j ($V_{min}^{i/j}$). The straight lines between the peaks and knots are distribution boundaries. At a boundary, a component is at the limit of appearing or disappearing in one of the product streams. We denote the distribution regions by the components being distributed to both products when operating in that region. For example in region AB components A and B are distributing to both products, whereas component C only appear in the bottom product. In region ABC all three components distribute to both products. At Point P_{AC},

the preferred split[2], only the intermediate component B distributes. The light A appears only in the top and the heavy C only in the bottom, and both A and C are exactly at the limit of being distributed. In regions A, B and C we have non-optimal operation with $V > V_{min}$. All the possible minimum energy solutions ($V = V_{min}$) are found below the "mountain", in regions AB, ABC or BC. There is an unique minimum energy solution fore each feasible pair of a key component specification in the top and in the bottom. Note that the active common Underwood roots are those in the range between the volatilities of the distributing components, and that no roots are active in the non-optimal regions above the "mountain".

In the following we show how to use the V_{min}-diagram for directly coupled columns like the Petlyuk arrangement.

3   The Underwood Equations Applied to Directly Coupled Sections

3.1   The Petlyuk Column Prefractionator

In the prefractionator of a Petlyuk column we can still use the net component flow (w) to describe the separation carried out in the column. From the material balance at any cross-section in the column:

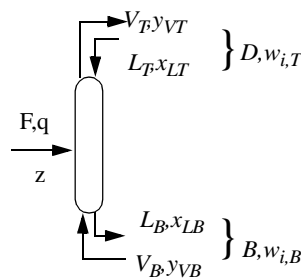$$w_{i,n} = V_n y_{i,n} - L_{n+1} x_{i+1,n} \qquad (4)$$

Figure 3: The prefractionator
of a Petlyuk arrangement.

Thus, for the column in Figure 3 the composition in the flow leaving the column top is dependent on the composition of the incoming flow through the material balance:

$$y_{i,VT} = \frac{w_{i,T} + L_T x_{i,LT}}{V_T} \tag{5}$$

For a conventional column with total condenser we have $x_{i,LT} = y_{i,VT}$, and $y_{i,LT} = w_{i,T}/D$, where $D = V_T - L_T$, but this does not apply here. However, even if there are external streams entering into the top and bottom, the composition in these streams do normally not affect the distribution of the feed components (w_i) to the top and bottom in the column and the following rule[8] can be used:

The V_{min}-diagram for a conventional column can also be applied to the Petlyuk prefractionator, provided that a component, that would have been removed from one end in the conventional column, does not appear in the end "feeds" of the Petlyuk prefractionator.

3.2 "Carry Over" of Underwood Roots in Directly Coupled Columns

The first part of this section is mainly based on Carlberg and Westerberg[6,7] who pointed out that Underwood roots "carry over" from the top of the first columns to the second column in the directly- or fully thermally coupled columns as shown in Figure 4.
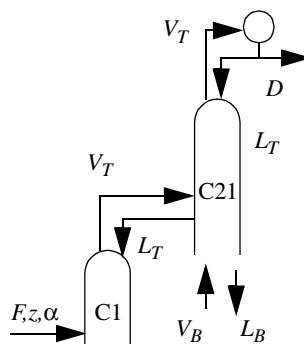

Figure 4: Directly coupled columns (fully thermally coupled).

The vapour flow in the top of the prefractionator is given by the Underwood defining equation:

$$V_T^{C1} = \sum_i \frac{\alpha_i w_{i,T}^{C1}}{\alpha_i - \phi^{C1}} \tag{6}$$

Note that we generally have to apply the actual Underwood roots (ϕ). The common roots (θ) only apply for minimum energy operation.

The top and bottom defining equations (2) for column C21 become:

$$V_T^{C21} = \sum_i \frac{\alpha_i w_{i,T}^{C21}}{\alpha_i - \phi^{C21}} \quad \text{and} \quad V_B^{C21} = \sum_i \frac{\alpha_i w_{i,B}^{C21}}{\alpha_i - \psi^{C21}} \tag{7}$$

The material balance at the connection point gives:

$$V_T^{C21} - V_B^{C21} = V_T^{C1} \quad \text{and} \quad w_{i,T}^{C21} - w_{i,B}^{C21} = w_{i,T}^{C1} \tag{8}$$

The combination of these gives the feed equation (3) for column C21 where the common roots (θ^{C21}) appear:

$$V_T^{C21} - V_B^{C21} = \sum_i \frac{\alpha_i(w_{i,T}^{C21} - w_{i,B}^{C21})}{\alpha_i - \theta^{C21}} = \sum_i \frac{\alpha_i w_{i,T}^{C1}}{\alpha_i - \theta^{C21}} = V_T^{C1} \tag{9}$$

Here we observe that the feed equation of column C21 (9) is identical to the top section defining equation for column C1 in (6). Thus the possible common roots in column C21 are equal to the actual roots from the defining equation in the top of column C1[6,7]:

$$\theta^{C21} = \phi^{C1} \tag{10}$$

Assume that we recover all the light A in the top of column C21. Then $w_{A,T}^{C21} = z_A F$, $w_{B,T}^{C21} = w_{C,T}^{C21} = 0$. The minimum vapour flow in column C21 for any given operation of C1 is when the common root (θ_A^{C21}) is active, which implies $\phi_A^{C21} = \theta_A^{C21} = \phi_A^{C1}$ and from (2) we have:

$$\frac{V_{Tmin}^{C21}}{F} = \frac{\alpha_A z_A}{\alpha_A - \phi_A^{C1}} \tag{11}$$

where $F = F^{C1}$ and z is the feed composition to column C1. Since $\theta_A^{C1} \le \phi_A^{C1}$, the absolute minimum solution is found when $\phi_A^{C1} = \theta_A^{C1}$. Then the common root of C1 becomes active in both column C1 and C21 at the same time ($\phi_A^{C21} = \theta_A^{C21} = \phi_A^{C1} = \theta_A^{C1}$) and:

$$\min_{C1}\left(\frac{V_{Tmin}^{C21}}{F}\right) = \frac{\alpha_A z_A}{\alpha_A - \theta_A^{C1}} \tag{12}$$

As usual the notation "V_{min}" represents the minimum vapour flow for a single column for a given feed. The outer "$min()$" represents the effect of the operation of column C1 to the feed composition and the effective feed quality for column C21. The common roots (θ^{C1}) are given by the feed equation (3) for the main feed to column C1.

We may generalize this expression to any number of components and feasible recoveries of components from the main feed in the top of column C21 with the following equation set (one equation for each active Underwood root in column C1 $\theta_k \in [\theta_1 \dots \theta_{N_{dT}^{C21} - 1}]$ given by the N_{dT}^{C21} components distributed to the top of C21):

$$\min_{C1}\left(\frac{V_{Tmin}^{C21}}{F}\right) = \sum_{i=1}^{N} \frac{\alpha_i w_{i,T}^{C21}}{\alpha_i - \theta_k^{C1}} \tag{13}$$

For column C22 connected to the bottom of column C1, we have equivalent results. For the ternary feed case, with full recovery of the heavy component C in the bottom of column C22 and zero recovery of the middle and light components, the equivalent to equation (12) is:

$$\min_{C1}\left(\frac{V_{Bmin}^{C22}}{F}\right) = \frac{-\alpha_C z_C}{\alpha_C - \theta_B^{C1}} = \frac{\alpha_A z_A}{\alpha_A - \theta_B^{C1}} + \frac{\alpha_B z_B}{\alpha_B - \theta_B^{C1}} - (1 - q) \tag{14}$$

Note that we have not considered the actual compositions in the junction streams. However, we know from Section 3.1[8], that the composition in the return flow into the top of C1 has no influence on the product split in C1 unless a component which would have been removed in a conventional prefractionator were to be introduced in that return flow. This implies that for nonsharp operation of C1, (where all components distribute and all common roots are active) the return-flow composition has no influence at all. For preferred split operation, this is also true when we ensure that there is no heavy (C) component in the return flow from C21 to C1.

In normal operation regimes of C1 and C21, the conditions are trivially fulfilled.

4   Minimum Energy for Separating a Ternary Feed in a Petlyuk Arrangement

We here consider the separation of a ternary feed mixture (components A,B and C) in the three-product Petlyuk arrangement in Figure 1. In the following, all Underwood roots (θ, ϕ, ψ) without superscript are related to column C1 or an equivalent two-product column with the same feed.

4.1   Coupling Column C22 with Columns C21 and C1

For a sharp A/C split in column C1 and sharp A/B split in column C21, minimum vapour flow requirement in the top of C21 is given by equation (11):

$$V_T^{C21} \geq V_{Tmin}^{C21} = \frac{\alpha_A z_A}{\alpha_A - \phi_A} F \tag{15}$$

We can also find the equivalent for the bottom flow in C22 for sharp B/C split from equation (14):

$$V_B^{C22} \geq V_{Bmin}^{C22} = \frac{-\alpha_C z_C}{\alpha_C - \psi_C} F \tag{16}$$

Due to the direct coupling we know that the absolute minimum vapour flow in C21 is found when we operate column C1 in a region where $\phi_A = \theta_A$. Similarly, the absolute minimum for vapour flow in C22 is found when C1 is operated in a region where $\psi_C = \theta_B$. For sharp product splits, the preferred split is the only point of operation where <u>both</u> common roots carry over to C21 and C22 at the same time. (Any other solution will give a larger value for the minim vapour flow in at least one of C21 or C22).

The Petlyuk arrangement has a single reboiler and the flow there must exceed the demands from both column C21 and C22. Thus we have:

$$V_{Bmin}^{Petl} = \max\left(\min_{C1} (V_{Tmin}^{C21}) - (1-q)F, \min_{C1} (V_{Bmin}^{C22})\right) \tag{17}$$

For sharp product splits, we can express this as:

$$V_{Bmin}^{Petl} = \max\left(\frac{\alpha_A z_A}{\alpha_A - \theta_A} - (1-q), \frac{-\alpha_C z_C}{\alpha_C - \theta_B}\right)F \tag{18}$$

or equivalently for the top of the Petlyuk arrangement:

$$V_{Tmin}^{Petl} = V_{Bmin}^{Petl} + (1-q)F = max\left(\frac{\alpha_A z_A}{\alpha_A - \theta_A}, \frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{\alpha_B z_B}{\alpha_B - \theta_B}\right)F \tag{19}$$

This expression (19) is identical to equation (1) of Fidkowski and Krolikowski[3], but (19) is more general in that it is also valid for an arbitrary feed quality (q). Note from (3) that q affects the solution for the common Underwood roots (θ_A, θ_B) and not only the term $(1-q)F$.

At this minimum solution either C21 or C22 may get a vapour flow larger than its minimum. However, this only affects the local behaviour of that column, and not the product composition and the operation of the prefractionator and the other column (ref Section 3.1).

4.2   Visualization in the V_{min}-diagram

By a closer inspection of the vapour flow rates for the Petlyuk arrangement, we observe that all the impor-

tant information can be found in the V_{min}-diagram for the feed to the prefractionator (C1). Figure 5 illustrates this

for a ternary example. The expressions for the peaks P_{AC}, P_{BC} (and also the preferred split P_{AC}) for a ternary feed

are given by Underwood's equations (Part I[8]). In P_{AB} we recover all the light A component ($w_{A,T} = z_A F$) and

θ_A is active. In P_{BC} we recover all of both A and B and θ_B is active, thus get from (2) and (3):

$$P_{AB}: \quad \frac{V_{Tmin}^{C1,A/B}}{F} = \frac{\alpha_A z_A}{\alpha_A - \theta_A} \tag{20}$$

$$P_{BC}: \quad \frac{V_{Tmin}^{C1,B/C}}{F} = \frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{\alpha_B z_B}{\alpha_B - \theta_B} \tag{21}$$

These are exactly the same terms as the expression for V_{Tmin}^{Petl} in equation (19) (the notation i/j in the super-

script denotes sharp i/j-split in a two-product column), that is:

$$V_{Tmin}^{Petl} = max(V_{Tmin}^{C1,A/B}, V_{Tmin}^{C1,B/C}) \tag{22}$$

Similarly we find for the vapour flow requirement into the bottom of the Petlyuk column:

$$V_{Bmin}^{Petl} = max(V_{Bmin}^{C1,A/B}, V_{Bmin}^{C1,B/C}) \tag{23}$$

This leads to the following important conclusion for pure product specifications:

The minimum vapour flow rate requirement in the Petlyuk column with three pure products is the same as

the minimum vapour flow for the most difficult of the two sharp component splits A/B or B/C in a single

conventional distillation column.

This is illustrated in the equation below where we use the column drawings as superscripts (the Petlyuk

column is shown as a dividing wall column).

$$
\begin{array}{c}
\text{[column diagram }V_{Bmin}^{\;\;C}\text{]}
\end{array}
= \; Max \left(\begin{array}{cc}
\text{[column }V_{Bmin}^{\;\;BC}\text{]} & \text{[column }V_{Bmin}^{\;\;C}\text{]} \\
\end{array} \right)
\tag{24}
$$

In the V_{min}-diagram this conclusion is the same as:

The minimum energy of a Petlyuk arrangement is characterized as the highest peak in the V_{min}-diagram.

Thus, for the case shown in Figure 5 we observe by a glance at the diagram that P_{BC} is the highest peak and thereby $V_{Bmin}^{Petl} = V_{Bmin}^{B/C}$.

We may also read the required minimum vapour flows in all sections of the Petlyuk arrangement directly from the V_{min}-diagram for the prefractionator feed as shown in Figure 5. The relations are trivial to derive from the material balance at the junctions.
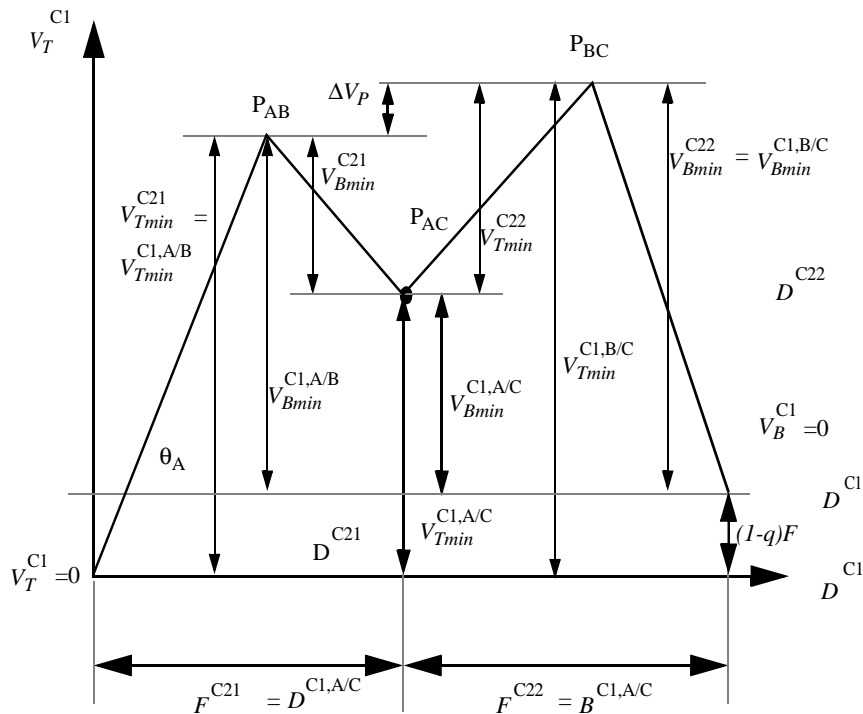

Figure 5: Use of the V_{min}-diagram for assessment of a Petlyuk arrangement.

4.3   The Flat Optimality Region

When we consider the preferred split operation we have in general three different solution cases, characterized by the requirement for minimum vapour flow from column C21 and C22 in the main column:

1. C22 controls: $V_{Bmin}^{C22} > V_{Tmin}^{C21} - (1-q)F$ or $V_{Bmin}^{C1,A/B} < V_{Bmin}^{C1,B/C}$

2. Balanced: $V_{Bmin}^{C22} = V_{Tmin}^{C21} - (1-q)F$ or $V_{Bmin}^{C1,A/B} = V_{Bmin}^{C1,B/C}$

3. C21 controls: $V_{Bmin}^{C22} < V_{Tmin}^{C21} - (1-q)F$ or $V_{Bmin}^{C1,A/B} > V_{Bmin}^{C1,B/C}$

In Cases 1 and 3, there are different vapour flow requirements in bottom of C21 and top of C22. The difference is given directly as the difference between the height of the peaks in Figure 5. For a balanced main column (Case 2) the peaks are equal. The highest peak always sets the overall requirement.

When we implement the vapour flow in the reboiler we simply use:

$$V_B^{C22} = V_{Bmin}^{Petl} \tag{25}$$

and in the top we have

$$V_T^{C21} = V_{Bmin}^{Petl} + (1-q)F \tag{26}$$

Let us now assume we have the situation in Case 1. It is obvious that since $V_T^{C21} > min(V_{Tmin}^{C21})$, the root θ_A cannot be active in C21. The amount of distillate product is the total amount of A from the feed, and we have the following defining equation with this specification, from which we can solve for the root.

$$V_T^{C21} = \frac{\alpha_A z_A F}{\alpha_A - \phi_{Abal}^{C21}} = V_{Bmin}^{Petl} + (1-q)F \tag{27}$$

We have two limiting cases. The first is when we operate the prefractionator at the preferred split. Then θ_A is active in C1, and since it will carry over to the feed equation in C21 we clearly waste vapour flow in C21. The other limiting case is when we move the operation point of C1 along the boundary BC/B until $\phi_A^{C1} = \phi_{Abal}^{C21}$. In this case the vapour flow in C21 is a local V_{min} solution in C21, thus $V_T^{C22} = V_{Tmin}^{C21} > min(V_{Tmin}^{C21})$. Now the main column is balanced since:

$$V_T^{C22} = V_{Tmin}^{C22}(D^{C1}, V^{C1}) = V_{Bmin}^{C21}(D^{C1}, V^{C1}) = V_B^{C21} \tag{28}$$

Outside this flat optimality region, the overall vapour flow requirement increase rapidly. Figure 6 gives an example where we have plotted the balance point, and also shows how the overall minimum vapour flow for the Petlyuk column depends on the prefractionator net product flow (D).
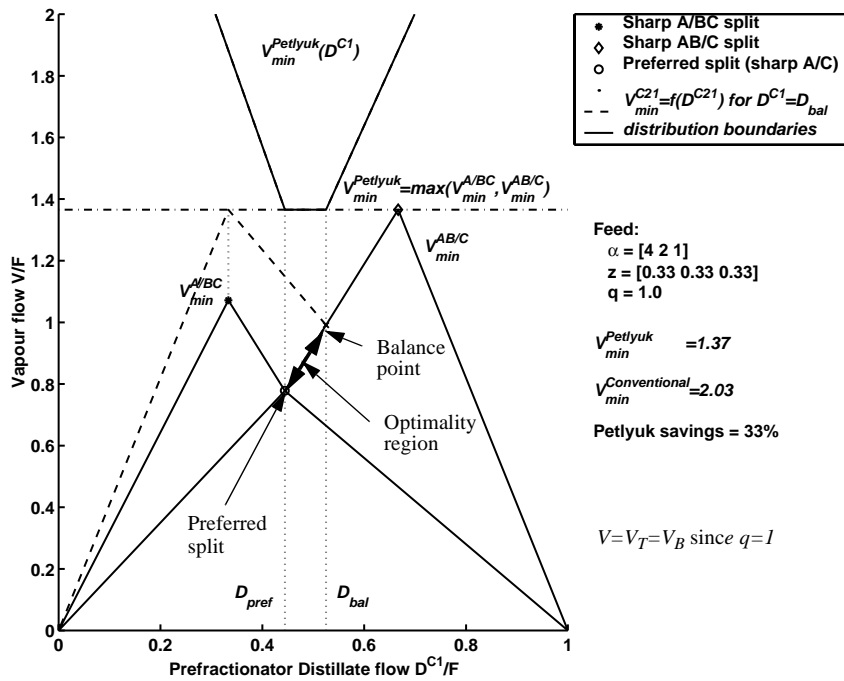

Figure 6: V_{min} for the prefractionator (C1) and the overall Petlyuk column (with flat optimality region) as a function of D/F for the prefractionator.

In this example, we may find the real root (ϕ_{Abal}) in the top of C1, (which carries over to C21) related to the balance point from:

$$\frac{V_{Tmin}^{Petl}}{F} = \frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{\alpha_B z_B}{\alpha_B - \theta_B} = \frac{\alpha_A z_A}{\alpha_A - \phi_{Abal}} \tag{29}$$

Knowing ϕ_A and $\phi_B = \theta_B$ in the balance point, we find the actual D and V for the prefractionator directly from the defining equations for the Underwood roots. The V_{min}-diagram for C21 when $\phi_A = \phi_{Abal}$ is shown dashed in Figure 6.

If the peak P_{AB} were the highest, we would have a Case 3 situation, with the optimality region to the left of the preferred split. We may summarize

The flat optimality region is found from the preferred split and on the V-shaped minimum energy boundary for sharp A/C split towards the highest peak. The extent of the optimality region depends on the difference of the height of the peaks, or in other words; the difference in how difficult it is to separate A/B or B/C in a single column.

4.4   Nonsharp Product Specifications

For nonsharp specifications the minimum vapour flow in the top section of column C21 is given from (13) when the net component flows in the top product is known. In the ternary case where both A and B may appear in the top and both B and C in the bottom, the generalization of (15) and (16) becomes:

$$V_{Tmin}^{C21} = \frac{\alpha_A w_{A,T}^{C21}}{\alpha_A - \theta_A} + \frac{\alpha_B w_{B,T}^{C21}}{\alpha_B - \theta_A} \tag{30}$$

$$V_{Bmin}^{C22} = \frac{\alpha_B w_{B,B}^{C22}}{\alpha_B - \theta_B} + \frac{\alpha_C w_{C,B}^{C22}}{\alpha_C - \theta_B} \tag{31}$$

where the net flows are obtained from the product specifications. These results represent the minimum energy in a single column for the splits of the top/middle and middle/bottom products respectively, just as in the sharp split case. The overall requirement is determined by the one giving the highest reboiler requirement according to equation (17).

Nonsharp product specifications for the ternary feed case have been treated in full detail in Chapter 9 of Halvorsen[8] where we show that the nonsharp sidestream impurity specification actually extends the optimality region from a line segment to a quadrangle in the plane spanned by the two selected degrees of freedom.

5 Multicomponent Feed

We here extend the results from the previous section to more than 3 feed components. The minimum energy is still be given by the largest minimum energy requirement from either column C21 or C22 as in equation (17).

First note that the Underwood roots carry over from the prefractionator to columns C21 and C22 in the same way for any number of components in the feed. This implies that if we operate the prefractionator at its preferred split, all the common underwood roots carry over. The general expression in equation (13) covers both multicomponent feed and nonsharp separations. However, this implies that the V_{min}-diagrams for columns C21 and C22 will overlap the diagram for column C1 also in the multicomponent case. Note that the V_{min}-diagram is based solely on the properties of the feed to column C1 and characterise distribution regions in an ordinary 2-product column. The fact that we can use the same diagram for the whole Petlyuk arrangement is very important and gives us a powerful and simple tool for assessment of any given separation task in a Petlyuk arrangement.

5.1 General Rule

We extend the rule given in Section 4.2 for a ternary feed and sharp component splits, to a general multicomponent feed and three composite and possible nonsharp product specifications:

The minimum vapour flow requirement in the Petlyuk column with three products is the same as the minimum vapour flow for the most difficult of the two possible product splits (top/middle- or middle/bottom-products) in a single conventional distillation column.

This is characterized as the highest peak in the resulting V_{min}-diagram for the products.

We simply replaced the term "component" from Section 4.2 with "product".

To obtain analytical solutions for minimum vapour flow and product splits we apply the computational tools based on the Underwood equations presented in Part I[8,9].

Two examples, with *N=5* components (ABCDE) in the feed, are now used to illustrate how simple it is to use the V_{min}-diagram to find the minimum energy solution and flow requirements in the Petlyuk arrangement. We do not give any particular feed properties, thus the diagrams should be interpreted qualitatively.

5.2 Example: Sharp Separations

First consider a case where we want AB in the top product, CD in the sidestream and pure E in the bottom. A V_{min}-diagram is shown in Figure 7.

In the prefractionator we have to remove AB from the bottom and E from the top. This is obtained along the "V"- shaped boundary P_{BC}-P_{BD}-P_{BE}-P_{CE}-P_{DE} (solid bold). The "preferred" solution for the prefractionator is to operate at P_{BE}. In column C21 know that the diagram for C21 overlap the diagram for C1 to the left of the preferred split when column C1 is operated at the preferred split. Column C21 shall perform a sharp AB/C separation and the minimum energy solution then simply found at P_{BC}. Similarly, in column C22 the peak P_{DE} gives the corresponding minimum vapour flow for sharp split between CD/E. Thus the Petlyuk arrangement requirement is simply given by the highest peak P_{BC} or P_{DE}, which is the encircled P_{BC} in the figure.
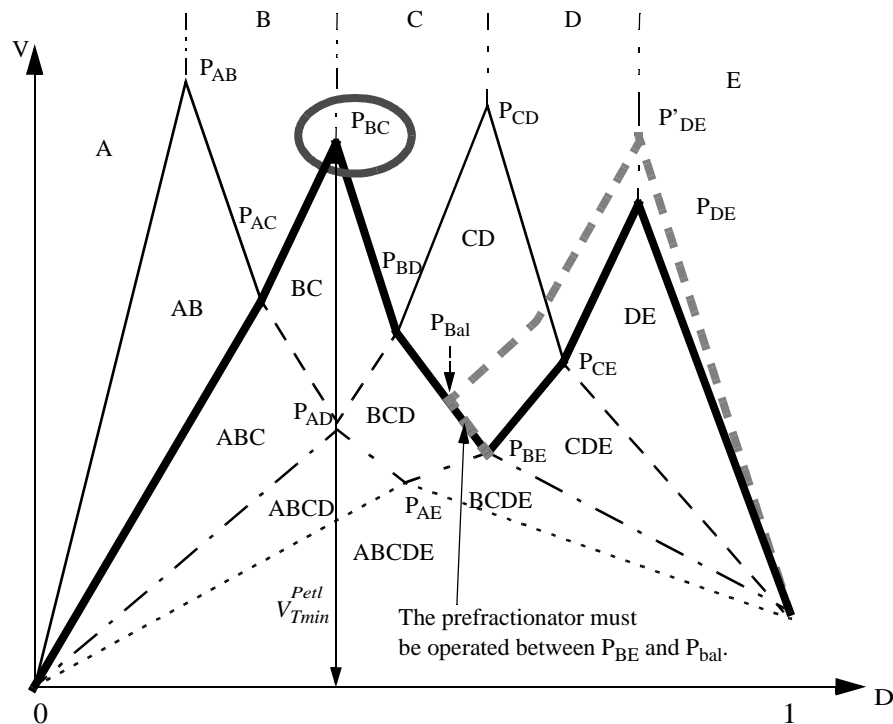
Figure 7: V_{min}-diagram for 5 component feed used to find minimum vapour flow requirements in a 3 product Petlyuk arrangement for sharp product splits AB/CD/E.

In this case we will also have a flat optimality region. It is shown qualitatively that if we move the operation of column C1 to the left of the preferred split, along the boundary BCD/CD, the peak P_{DE} will start to increase. At P'_{DE} it becomes equal to P_{BC} and the main column is balanced, and the prefractionator (C1) is operated at P_{bal}. Thus, minimum vapour flow for the Petlyuk column can be obtained only when the prefractionator is operated along the line between P_{BE} and P_{bal}.

Note that a peak in the V_{min}-diagram is simply the vapour flow requirement for a particular sharp split in an ordinary two-product column. Thus the minimum vapour flow requirement for the Petlyuk arrangement is given by most difficult split between two of our specified product groups, if the separation was to be carried out in a conventional 2-product column.

This is illustrated in "equation" (32). In this example P_{CD} is an higher peak than P_{BC} or P_{DE}, but this does not matter since we do not attempt to split the D and C components into separate products (subscript T,B is not used since we may consider either tops or bottoms).

$$
\begin{matrix} \text{AB} \\ \text{CD} \\ \text{E} \\ V_{min} \end{matrix} \quad = \quad \text{Max} \left(\begin{matrix} \text{AB} \\ \text{CDE} \\ V_{min} \end{matrix} \, , \quad \begin{matrix} \text{ABCD} \\ \text{E} \\ V_{min} \end{matrix} \right) \tag{32}
$$

5.3 Example: Nonsharp Separations

In the next example, as shown in Figure 8, we use the same feed and V_{min}-diagram, but we change the product specifications so that all the light A component is recovered in the top, all the C component in the sidestream and all heavy E in the bottom. However, in this case we allow B to appear in both top and sidestream products, and D to appear in both the sidestream and bottom products.
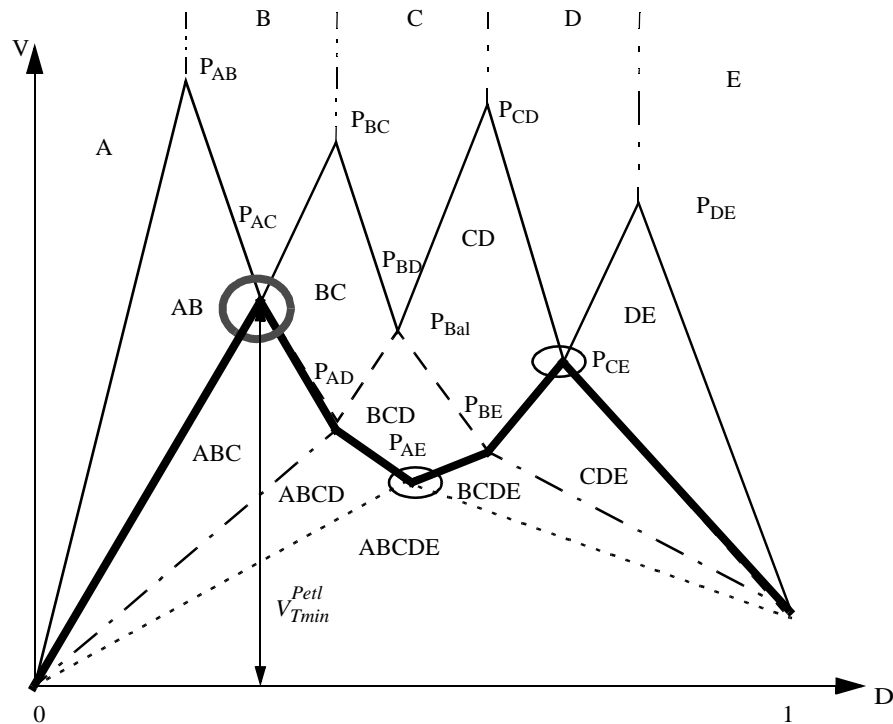

Figure 8: V_{min}-diagram for 5 component feed used to find minimum vapour flow requirements in a 3 product Petlyuk arrangement. Specification with nonsharp product splits AB/BCD/DE.

The solution is still quite simple to obtain from the V_{min}-diagram. In the prefractionator we need to remove A from the bottom and E from the top, and the minimum vapour flow in the prefractionator is found at the preferred split P_{AE}. This time all common roots carry over, and C21 and C22 becomes columns with 4-component

feeds. However, the interesting point of operation in column is the sharp split between A and C. Since both θ_A, θ_B carry over from C1, the minimum vapour flow in the top of C21 is trivially found at P_{AC}. Similarly P_{CE} will give the requirement in C22. Again, the separation is found to be exactly the same as the most difficult product split when we compare one and one such split in an ordinary 2-product distillation column as shown in "equation" (33).

$$\left. \begin{array}{c} \text{AB} \\ \text{BCD} \\ V_{min} \quad \text{DE} \end{array} \right| = \quad \text{Max} \left(\begin{array}{cc} \text{AB} & \text{ABCD} \\ \text{BCDE} & \text{DE} \\ V_{min}, & V_{min} \end{array} \right) \tag{33}$$

Note that in both these examples, the bold lines represent minimum energy solution for sharp split between a pair of the specified (composite) products in either top or bottom of an ordinary two-product column.

6 Discussion

6.1 Improved 2nd Law Results in Petlyuk Arrangements

Several authors e.g. Carlberg and Westerberg[7], Agrawal and Fidkowski[14], Annakou and Mizsey[15], mention that a typical Petlyuk column, where all the heat input is done at the highest temperature level, and all the heat removal is done at the lowest temperature level, has a drawback compared to conventional arrangements where some heat is added and removed at intermediate levels. Even if the overall vapour flow rate, which can be regarded as a first law (of thermodynamics) effect, is always less than in a conventional arrangement[16], the temperature range between heat input and removal is always the largest boiling point difference, which gives low performance in terms of the second law effect. Thus, in order to recommend a Petlyuk arrangement, the first law effect must dominate over the second law effect with respect to the utility requirement.

However, when the peaks in the V_{min}-diagram are of different height, this implies that a change in vapour flow could be allowed at the sidestream stage. In the case when the vapour flow requirement in the lower end is larger, this may easily be realised by extracting some of the sidestream product as vapour. This may be done either directly, or by withdrawing all the liquid from C21 and returning it slightly cooled, exactly sufficient to condense

the required change in vapour at the return stage. In cases where the vapour flow in C21 is higher, some of the heat can be supplied at the sidestream stage. The maximum flow rate is still given by the highest peak, but not all of it has to be supplied or removed at the most extreme temperatures.

A heat exchanger at the sidestream stage as illustrated in Figure 9 can ensure that both C21 and C22 are operated at minimum energy at the same time. The actual change in vapour flow can easily be found from the V_{min}-diagram as the difference height of the two peaks P_{AB} and P_{BC} (see ΔV_P in Figure 5). The prefractionator now has to be operated exactly at its preferred split.
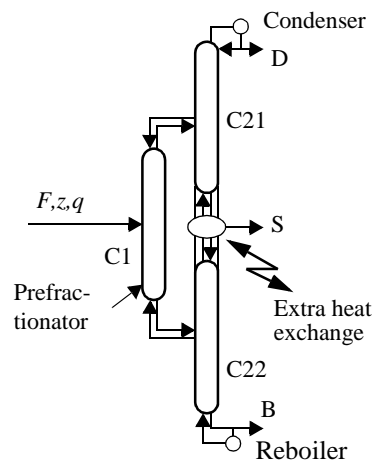

Figure 9: Petlyuk arrangement with extra heat exchange at the sidestream stage.

The cases where the second law effect cannot be improved is for a balanced main column. Then the vapour flow requirements are the same in the top and bottom and this is also the case where we obtain the largest vapour flow rate savings, compared to the best of conventional direct or indirect split configurations (ref. Chapter 8 of Halvorsen[8]). In these cases the first law effect is most likely to dominate over the second law effect.

We have not done a detailed comparative study with other types of columns and heat integration, taking a heat exchanger at the sidestream stage into consideration, but it is clear that some results in other studies[14,15], would have been more favourable for a Petlyuk arrangement if this extra heat exchange ability had been included.

6.2   Composition Profiles

An operational and computational advantage with the directly connected prefractionator is that we may decouple the feed split, expressed by the net flow of each component ($w_{i,T}$), from the composition in the flow leaving the column. In Figure 10 the profiles for the preferred split are shown for a Petlyuk column prefractionator a), and a conventional column b). The end-feed compositions have been set equal to the pinch zone compositions in each end of the Petlyuk prefractionator. This implies that the vapour and liquid compositions in each end are at equilibrium and these will also be the feed pinch composition of the succeeding columns when the Petlyuk arrangement is operated at minimum energy.

The differences between the conventional and directly coupled column are observed towards the ends. In the conventional columns remixing occurs caused by recycling of the condenser and reboiler products.
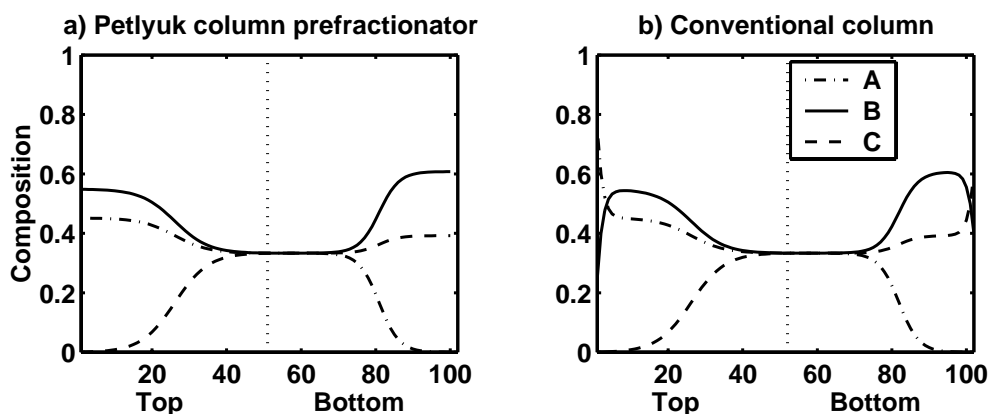

Figure 10: Composition profiles at preferred split. Feed data z=[0.33 0.33 0.33], α =[4 2 1], q=1. End feeds in a) are set equal to pinch zone compositions.

6.3   Non-optimal Operation

In case of operation of the prefractionator outside the flat optimality region of the Petlyuk arrangement, the energy requirement increases rapidly[17]. In some cases we may get recycling of net flow of the intermediate component from either column C21 or column C22 back into the prefractionator column. This violates Underwood's assumption about positive net flow of components from the feed to each of the product ends as discussed in Section 3.1. However, with some constraints on the composition in the liquid entering at the top or the vapour into

the bottom, we may still use Underwood's equations to compute the minimum vapour flow solutions for all parts of the arrangement. This issue is treated in more detail in the thesis by Halvorsen[8] also for non-sharp product specifications.

6.4 Extra Condenser or Reboiler in the Prefractionator

Several authors, e.g. Agrawal and Fidkowski[14] have pointed out that in some cases, the overall minimum vapour flow rate may be unaffected if a condenser is used at the prefractionator top as shown in Figure 11. This is very simple to asses by the V_{min} diagram. The effect of introducing a prefractionator condenser is that the vapour requirement in column C21 increases. In order to obtain the same minimum boilup requirement, first the peak P_{BC} has to be the highest peak, and second, the difference between the peaks have to be larger than the additional vapour requirement in column C21 imposed by a (possibly partial) condenser on the top of column C1.
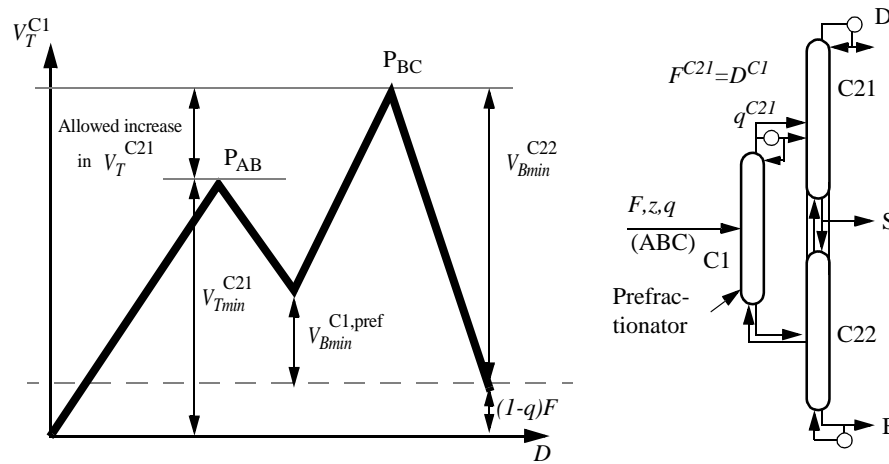

Figure 11: The V_{min}-diagram for the 3-component feed (ABC) gives directly the allowed increase in the vapour flow in column C21. The modified Petlyuk arrangement may then obtain the same minimum reboiler flow as the full Petlyuk arrangement, given by P_{BC}.

Similarly, a combined arrangement with a direct coupling between column C1 and C21 and a reboiler at the bottom of C1 and conventional feed to C22, may require the same total minimum vapour flow as a Petlyuk arrangement only if the peak P_{AB} is significantly higher than P_{BC}.

6.5 Use of a Conventional Prefractionator Column

A configuration with a conventional prefractionator column with its own reboiler and condenser as shown in Figure 12 was studied by Christiansen[18]. This approach may in some cases come close to the Petlyuk arrangement in terms of overall vapour flow, but never better. In other cases, the minimum vapour flow will be higher than with the conventional configurations. Halvorsen[8] showed that the optimum is always found when the prefractionator is operated exactly at the preferred split. We will also have an operating point where the main column is balanced, but in the this case there is no completely flat optimality region since the total vapour flow with a balanced main column will always be slightly above the requirement at preferred split operation.
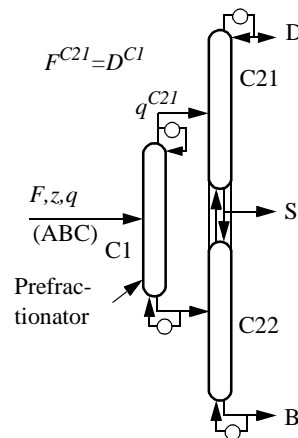

Figure 12: Conventional prefractionator arrangement.

6.6 Real Mixtures

As shown in Part I, a V_{min}-diagram can be made for real (zeotropic) mixtures. This implies that we may use the V_{min}-diagram for assessment of separation of real mixtures in the Petlyuk arrangement too. However, unlike in the ideal case where the V_{min}-diagram is a visualization of the exact analytical solution for minimum energy, we have to treat it as a tool that gives us approximate estimates, and the accuracy will of course be best for close to ideal mixtures. For more accurate computations we must adjust for changes in molar flows and other properties along the columns sections.

The main characteristics of the minimum energy solution is still (with reservations for some very non-ideal cases) that the prefractionator should be operated at its preferred split. This gives us the feed distribution in column C1 and thereby the feed stage conditions and the minimum energy requirements for the succeeding columns may easily be calculated numerically, for example in a rigorous process simulator.

7 Conclusion

The minimum energy solution for a 3-product Petlyuk arrangement has been analysed. The solution is given by the highest peak in the V_{min}-diagram for the feed, and this is equivalent to the following rule:

The minimum total vapour flow requirement in a Petlyuk arrangement is the same as the required vapour flow for the most difficult split between two of the specified products if that separation was to be carried out in a single conventional two-product column.

The V_{min}-diagram is based on feed data only, and in addition to the overall vapour flow requirement, we find the individual vapour flow requirement for each column section, directly from the same diagram as shown in Figure 5.

The plain Petlyuk arrangement will probably be most attractive when the peaks in the V_{min}-diagram are of similar height. Otherwise, combined arrangements may give similar performance in terms of minimum vapour flow, and even better performance in terms of separation work.

The minimum energy expression in itself is not a new result. However, the simple way to "see" the answer as "the most difficult binary split", the generalization to multicomponent feed and nonsharp product specifications and assessment by the V_{min}-diagram are hopefully useful contributions to the distillation literature. In this paper we have limited the analysis to 3-product Petlyuk columns, and we left an open question if a similar approach can be used for more then three products. We reveal that this is possible indeed, and the generalization to extended multi-product Petlyuk arrangements is the subject in Part III[19].

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