Optimal Operation of a Petlyuk Distillation Column: Energy Savings by Over-fractionating

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Abstract

This paper shows the unexpected result that over-fractionating one of the product streams in a Petlyuk distillation column may be optimal from a energy point of view. Analytic expressions for the potential energy savings are derived using the Underwood equations. The energy savings by over-fractionation may be further increased by bypassing some of the feed and mixing it with the over-fractionated product to meet product specifications. Normally, the energy savings are small, so the main significance of our results is to point out that over-fractionating is optimal in some cases.

1. Introduction

The Petlyuk distillation column, see Figure 1(a), with a pre-fractionator (C_1) and a main column (C_{21} and C_{22}), is an interesting alternative to the conventional cascade of binary columns for separation of ternary mixtures. The potential savings are reported to be of approximately 30% in both energy and capital cost (Smith and Triantafyllou 1992).

The feed (F) contain components A, B and C and enter the pre-fractionator with composition $\mathbf{z_f} = [z_{f,A}\ z_{f,B}\ z_{f,C}]^T$, liquid fraction q_f and relative volatility $\alpha = [\alpha_A\ \alpha_B\ \alpha_C]^T$. The column has three product streams, the bottom stream (B), the side stream (S) and the distillate (D). $x_{i,j}$ is the mole fraction of component i in stream j. The internal vapor and reflux flows are split (with split-factor R_v and R_l respectively) to the pre-fractionator and the main column.

In this work it is assumed that the operational objective is to minimize the energy consumption, which may be translated into minimizing the boilup V, while satisfying constraints on the composition of the main component in the three product streams. This formulation implicitly assume that all product streams have the same economic value. In mathematical terms, the operational objective becomes
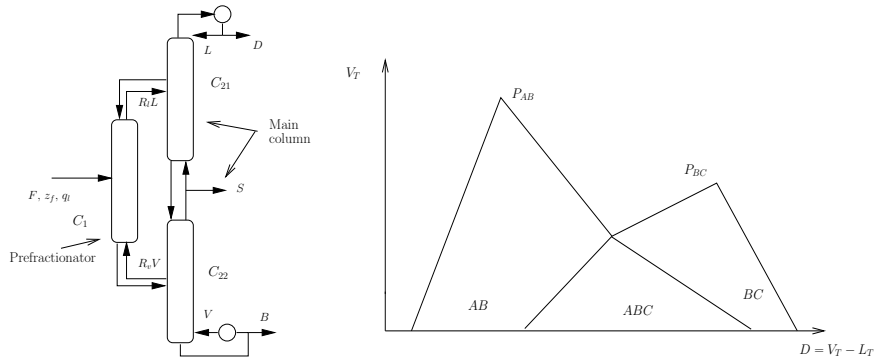
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$$\min_{\mathbf{u}} V \tag{1}$$

s.t.

$$x_{A,D} \geq x_{A,D}^0, \ x_{B,S} \geq x_{B,S}^0, \ x_{C,B} \geq x_{C,B}^0 \tag{2}$$

where $\mathbf{u} = [L \ V \ S \ R_l \ R_v]^T$ is the vector of steady-state degrees of freedom (manipulated inputs), and $x_{i,j}^0$ denote the minimum mole fraction of the main component $i \in \{A, B, C\}$ in each product stream $j \in \{D, S, B\}$. In addition we must require that all flows are positive.

(a) Sketch of the Petlyuk distillation column

(b) V_{min} diagram when C_{21} is limiting for a given feed. For the case when C_{22} is limiting, peak P_{BC} is above peak P_{AB}

Figure 1. Sketch and V_{min} diagram for the Petlyuk column

It is well known that when the products have different value, it may be economically optimal to over-fractionate the least valuable product in order to maximize the amount of the most valuable product. Here, we intend to show that there may be cases where it is optimal to over-fractionate one of the products to save energy. It is known from literature that for a conventional binary distillation column, bypassing a portion of the feed to the products does not affect the energy demand to produce the specified products (Bagajewich and Manousiouthakis 1992).

2. V_{min} Diagram and Underwood equations for the Petlyuk distillation column

The V_{min} diagram is a graphical representation of the energy requirements in distillation columns and provides an effective tool for analyzing the minimum energy requirements for different mixtures and feed properties (Halvorsen and Skogestad 2003). In this work we construct the V_{min} diagram from the Underwood equations (Underwood 1945) based on the assumption of constant molar flows, constant relative volatility and we assume infinite number of stages. For a three-product column it can be shown that the minimum

energy diagram for the Petlyuk column with sharp splits maps the V_{min} diagram for the pre-fractionator C_1 operated at the preferred split (Halvorsen and Skogestad 2003). Figure 1(b) shows the V_{min} diagram for the Petlyuk column with sharp splits. The peak P_{AB} corresponds to the split A/BC, while the peak P_{BC} corresponds to the split AB/C. The minimum energy is given by the highest peak, which corresponds to the most difficult separation. For non-sharp splits the same diagrams applies, but now with the vapor flows related to the non-sharp splits D/SB and DS/B, so the minimum energy for non-sharp splits is (Halvorsen and Skogestad 2003):

$$V_{T,min}^{Petl} = \max(V_{T,min}^{D/SB}, V_{T,min}^{DS/B}) = \max(V_{T,min}^{C_{21}}, V_{B,min}^{C_{22}} + (1-q_f)F) \tag{3}$$

where D, S and B here represents the three products with their defined compositions. Even for the case of non-sharp splits there will be no component C in the distillate ($x_{C,D} = 0$) and no component A in the bottom stream ($x_{A,B} = 0$) in normal operation regions. However, in the side-stream (S) all components may be present, and we chose $x_{A,S}$ as a free variable. Halvorsen and Skogestad (2003) show that three different regimes of operation is possible with accompanying optimal values for $x_{A,S}$:

- Case 1: C_{22} is limiting: This is the case when the separation B/C is the most difficult separation so peak P_{BC} is above peak P_{AB}, thus: $V_{T,min}^{Petl} = V_{B,min}^{C_{22}}(0) + (1 - q_f)F > V_{T,min}^{C_{21}}(1-x_{B,S})$ for $x_{A,S} = 0$ and $x_{C,S} = 1 - x_{B,S}$.

- Case 3: C_{21} is limiting This is the case when the separation A/B is the most difficult separation, as illustrated in Figure1(b) thus: $V_{T,min}^{Petl} = V_{T,min}^{C_{21}}(0) > V_{B,min}^{C_{22}}(1-x_{B,S}) + (1-q_f)F$ where $x_{A,S} = 1 - x_{B,S}$ and $x_{C,S} = 0$.

- Case 2: Balanced main column: This is when the required vapor load are equal: $V_{T,min}^{Petl} = V_{B,min}^{C_{22}}(x_{A,S}) + (1-q_f)F = V_{T,min}^{C_{21}}(x_{A,S})$ for $0 < x_{A,S} < 1 - x_{B,S}$ and $x_{C,S} = 1 - x_{B,S} - x_{A,S}$.

Halvorsen and Skogestad (2003) show that the vapor flows are given by

$$V_{T,min}^{C_{21}} = \frac{\alpha_A w_{A,T}^{C_{21}}}{\alpha_A - \theta_A} + \frac{\alpha_B w_{B,T}^{C_{21}}}{\alpha_B - \theta_A} = D\left[\frac{\alpha_A x_{A,D}}{\alpha_A - \theta_A} + \frac{\alpha_B(1 - x_{A,D})}{\alpha_B - \theta_A}\right] \tag{4}$$

and

$$V_{B,min}^{C_{22}} = \frac{\alpha_B w_{B,B}^{C_{22}}}{\alpha_B - \theta_B} + \frac{\alpha_C w_{C,B}^{C_{22}}}{\alpha_C - \theta_B} = -B\left[\frac{\alpha_A(1 - x_{C,B})}{\alpha_A - \theta_B} + \frac{\alpha_B(x_{C,B})}{\alpha_B - \theta_B}\right] \tag{5}$$

where $\theta_A = \theta_A(\mathbf{z_f}, q_f, \alpha)$ and $\theta_B = \theta_B(\mathbf{z_f}, q_f, \alpha)$ are the Underwood roots carried over from C_1 to C_{21} and C_{22} respectively, $w_{A,T}^{C_{21}} = x_{A,D}D$ and $w_{B,T} = x_{B,D}D = (1 - x_{A,D})D$ are the net component flow of A and B in C_{21} respectively, $w_{B,B}^{C_{22}} = -(1 - x_{C,B})B$ and $w_{C,B}^{C_{22}} = -x_{C,B}B$ are the net component flow of B and C in C_{22}. The key observation from (4) and (5) is that when $x_{C,B}$ is kept constant, $V_{T,min}^{C_{21}}/D$ is constant when C_{21} is limiting and when C_{22} is limiting, keeping $x_{A,D}$ constant implies $V_{B,min}^{C_{21}}/B$ constant. The only restriction is that C_{21} and C_{22} remain the limiting column section, respectively. With this observation, all that is needed to derive the results in this paper are the material balances.

3. Energy savings by over-fractionating

In the main column the same amount of vapor flows in sections C_{21} and C_{22}. This implies that when the column operates in either Case 1 or Case 3, the non-limiting section has a higher vapor flow than is necessary for the separation to take place. Thus, it is possible to over-fractionate in the non-limiting section without increasing the boil-up. Actually we can go even further and decrease the overall boilup. This is less obvious, so consider Case 1 where B/C is the most difficult separation (C_{22} is limiting). In this case we have excess vapor in the top of the main column (C_{21}) so the top product can be over-fractionated, for example, we can get pure A in the top product. The intermediate component B, that used to go in the top product, then goes into the side-stream product. The purity of the side-stream product can then be maintained by moving some (small) amount of component C from the bottom to the side-stream product. This results in a smaller bottom flow B and we can reduce V accordingly while keeping V/B constant. In conclusion we can thus reduce the boilup to the limiting bottom section by over-fractionating in the top.

3.1. Energy savings by over-purification, Case 1: C_{22} is limiting

To study this mathematically, the material balance of the column is given by (6)

$$
\begin{bmatrix} z_{f,A} \\ z_{f,B} \\ z_{f,C} \end{bmatrix} F =
\begin{bmatrix} x_{A,D} & x_{A,S} & 0 \\ (1-x_{A,D}) & x_{B,S} & (1-x_{C,B}) \\ 0 & (1-x_{B,S}-x_{A,S}) & x_{C,B} \end{bmatrix}
\begin{bmatrix} D \\ S \\ B \end{bmatrix}
\tag{6}
$$

where it is assumed that there is no heavy product in the top ($x_{C,D} = 0$) and no light components in the bottom stream ($x_{A,B} = 0$). Note that $x_{A,S} = 0$ for Case 1 when C_{22} is limiting. The reason for this is that it is optimal to introduce as much B into the side-stream as possible in order to reduce the boilup in the limiting section, thus moving A to the top. Therefore, when operating in Case 1 the constraints in (2) are given by $x_{B,S} = x_{B,S}^0$, $x_{C,B} = x_{C,B}^0$ and $x_{A,D} \geq x_{A,D}^0$.

From (6) we find that the bottom stream is given by

$$
B = -F \frac{\left(1 - \frac{z_A}{x_{A,D}}\right) x_{C,S} - z_C}{x_{C,B} - x_{C,S}}
\tag{7}
$$

From the mass balance equations it follows that when the fraction of component B is reduced in the distillate, we can transfer an amount $\Delta D = F z_A \frac{(1-x_{A,D}^0)}{x_{A,D}^0}$ to the side-stream S. To fulfill the side stream purity constraint we may then transfer an amount $\Delta B = \Delta D \frac{x_{C,S}^0}{x_{C,B}^0 - x_{C,S}^0}$ from the bottom stream to the side-stream. Further, it follows that the relative energy savings, when the purity is increased from the constraint value $x_{A,D}^0$ to $x_{A,D}$, is

$$
E_S^{C_{22}} = \frac{V_{B,min}^{C_{22},0} - V_{B,min}^{C_{22}}}{V_{B,min}^{C_{22},0}} = \frac{x_{C,S}^0 z_A \left(x_{A,D} - x_{A,D}^0\right)}{\left(z_A x_{C,S}^0 + z_C x_{A,D}^0 - x_{A,D}^0 x_{C,S}^0\right) x_{A,D}} = \frac{\frac{1}{x_{A,D}^0} - \frac{1}{x_{A,D}}}{\frac{z_C}{z_A} \frac{1}{x_{C,S}^0} + \frac{1}{x_{A,D}^0} - \frac{1}{z_A}}
\tag{8}
$$

Which is positive as long as $z_A x_{C,S}^0 + z_C x_{A,D}^0 - x_{A,D}^0 x_{C,S}^0 \geq 0$, this is usually the case since in practice $z_C > x_{C,S}^0$. From (8) we note that, lowering the purity requirement ($x_{A,D}^0$) will

increase the potential energy savings. Normally $\frac{z_C}{x_{C,S}^0} \gg 1$, so increasing z_A will also increase the energy savings, while increasing the amount of C in the side-stream S will reduce the energy savings. Normally $x_{A,D} = 1$ and $z_A x_{C,S}^0 + z_C x_{A,D}^0 - x_{A,D}^0 x_{C,S}^0 \approx 1$ (exact when $z_A = z_C$ and $x_{B,D}^0 = x_{C,S}^0$) so $E_S^{C22} \propto x_{C,S}^0 x_{B,D}^0$, the energy savings is proportional to the impurity specifications in the side-stream and the distillate.

3.2. Energy savings by over-fractionating, Case 3: C_{21} is limiting

For Case 3 the energy savings by over-fractionating the bottom product is

$$E_S^{C21} = \frac{V_{T,min}^{C21,0} - V_{T,min}^{C21}}{V_{T,min}^{C21,0}} = \frac{x_{A,S}^0 z_C \left(x_{C,B} - x_{C,B}^0\right)}{\left(z_A x_{C,B}^0 - x_{C,B}^0 x_{A,S}^0 + x_{A,S}^0 z_C\right) x_{C,B}} = \frac{\frac{1}{x_{C,B}^0} - \frac{1}{x_{C,B}}}{\frac{z_A}{z_C} \frac{1}{x_{A,S}^0} + \frac{1}{x_{C,B}^0} - \frac{1}{z_C}} \tag{9}$$

4. Additional energy savings by introducing bypass

Over-fractionating one of the product streams makes it possible to bypass some of the feed and mixing it into the product while retaining the constraints on the products as given by (2). For Case 1 (see Figure 2(b)), assume that we over-fractionate the distillate stream to pure A ($x_{A,D} = 1$). The resulting distillate flow is then $D = z_A F$ (remember $x_{A,S} = 0$). The amount of feed to bypass (F_B) is then given by (10)

$$F_B^{C22} = D(x_{B,D} = 0) \frac{x_{B,D}^0}{1 - x_{B,D}^0 - z_A} \tag{10}$$

To illustrate, Figure 2(a) shows the relative energy savings calculated as the reduction in boilup per feed unit with respect to $x_{D,D}^0$, when increasing the purity from $x_{A,D}^0$ to $x_{A,D} = 1$ for $\mathbf{z_f} = [0.5\ 0.3\ 0.2]$, $x_{B,B}^0 = 0.03$ and $x_{C,S}^0 = 0.1$. The dashed line indicates the potential savings when including bypass and the solid drawn line is with no bypass. A potential saving of approximately 4% is possible without bypass, while including a bypass increase the savings to approximately 13%.

For Case 3, when C_{21} is limiting we have that $x_{C,S} = 0$ optimally. Assume that the bottom stream is over-fractionated to pure component C, then $B = z_C F$ and the bypass is given by

$$F_B^{C21} = B(x_{B,B} = 0) \frac{x_{B,B}^0}{1 - x_{B,B}^0 - z_C} \tag{11}$$

5. Conclusion

In this paper it is has been shown that for Petlyuk distillation columns, it may be optimal from a energy point of view, to over-fractionate one of the product streams. Additional energy savings may also be possible when bypassing some of the feed and mixing it with the over-fractionated product stream. However, it should be noted that the distillate product will contain component C which may be undesirable. These results has been confirmed numerically for the case with finite number of stages, where it is optimal to over-fractionate the non-limiting section as expected. This implies that one may either choose to over-fractionate (in operation) or decrease the number of stages in the non-limiting section (design).
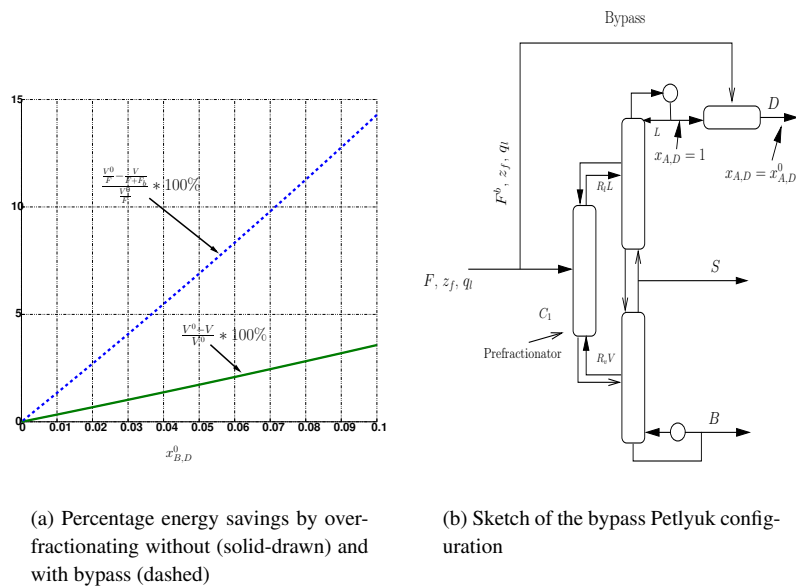
(a) Percentage energy savings by over-fractionating without (solid-drawn) and with bypass (dashed)

(b) Sketch of the bypass Petlyuk config-uration

Figure 2. Energy savings and sketch of the bypass Petlyuk configuration

6. References

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