

Shortcut Analysis of Optimal Operation of Petlyuk Distillation

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Analytical methods are used to compute important operational parameters for an infinite-staged Petlyuk column as a function of the feed composition, feed enthalpy, and relative volatilities. The computational effort is very low, and the methods can be used to quickly evaluate the applicability of a Petlyuk column for a specific separation task. It is found that the largest energy savings of about 40% are obtained when the prefractionator is operated at its preferred split and the feed composition is such that both the upper and lower parts of the main column operate at their respective minimum reflux condition. The position of this boundary region relative to the actual feed is very important when we consider important operational aspects of the column.

1. Introduction

The fully thermally coupled distillation arrangement¹ has several appealing features for separation of a three-component mixture. However, the industrial usage has been quite limited, even though it has been over 50 years since Wright's patent² (1949) for a dividing wall column. For a long time, the sole industrial exception has been BASF,³ which has several dividing wall columns in operation and is regarded as standard technology. More recently, Japanese,⁴ British,⁵ more German⁶ (outside BASF), American,⁷ and South African applications have been reported. Theoretical design studies and results from pilot-plant operation have been presented by Triantafyllou and Smith⁸ and Mutalib and Smith.⁹ Theoretical studies are presented by Agrawal and Fidkowski,^{10,11} Mizsey et al.,¹² and Dunneber and Pantelides.¹³ All authors report typical savings on the order of 30% in energy costs and that the implementation as a dividing wall column can also save considerable capital costs compared to traditional arrangements with two binary columns in series.

In this paper, we use analytical methods for infinite-staged high-purity columns. The methods^{14,15} can be used to quickly check if a Petlyuk arrangement is suitable for a particular separation case and indicate requirements for the level of automatic control and the design of the number of stages in each column section.

2. Petlyuk Distillation Column

The Petlyuk column, shown in Figure 1, separates a mixture of components, A–C. The column has at steady state 5 degrees of freedom that may be selected as the following manipulated input variables: boilup (V), reflux (L), midproduct side-stream flow (S), liquid split ($R_l = L_1/L$), and vapor split ($R_v = V_2/V$). As pointed out by Wollf and Skogestad,¹⁶ it is possible, in practice, to specify one product specification for each product: top (x_{DA}), bottom (x_{BC}), and side stream (x_{SA}). It is not

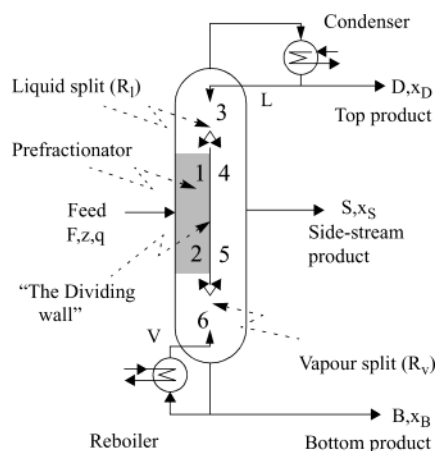


Figure 1. Petlyuk distillation arrangement implemented as a dividing wall column.

possible, in practice, to specify the relative amount of heavy and light impurities in the side stream. A very important issue is then that we have more degrees of freedom (5) than product specifications. The 2 extra degrees of freedom can be used for optimization purposes, such as to minimize the energy consumption. When the column is operated optimally, the infinite-staged Petlyuk column always consumes less energy than the corresponding conventional solution.¹⁷ However, this optimal operation may be difficult to achieve in practice because the optimal operation depends strongly on the feed properties and the remaining degrees of freedom.^{14,18}

In the following, we assume L , V , and S are used to control the product purities and let the liquid and vapor splits (R_l and R_v) be the remaining 2 degrees of freedom (note that other choices may be made). The overall energy consumption will then be a function of the degrees of freedom (R_l and R_v), the feed properties (z and q), and the product specifications (x_{DA} , x_{BC} , and x_{SB}). We choose to use the reboiler vapor flow V as a measure of the energy consumption.

Our aim is to adjust R_l and R_v in order to keep $V = V_{opt}$. The optimal values R_l and R_v can be found by minimizing the boilup with respect to the degrees of

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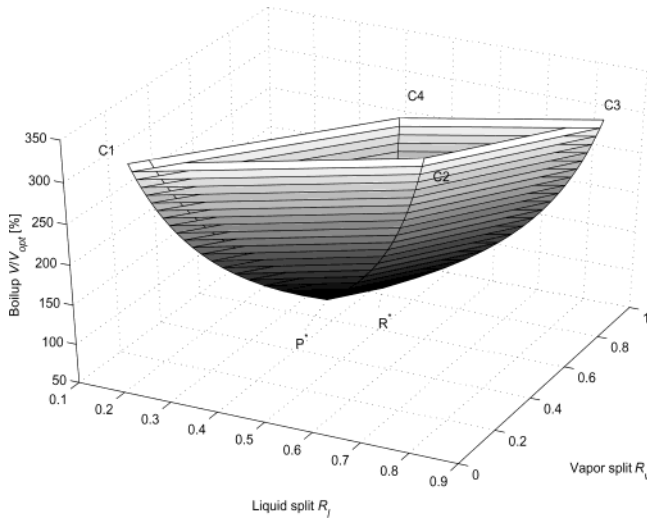


Figure 2. Solution surface $V(R_1, R_v)$ for the case with infinite stages and sharp splits.

freedom as shown in eq 1. The optimal boilup (V_{opt}) will be a function of the feed properties and product specifications.

An important observation for the Petlyuk column is that $V \approx V_{opt}$ for a broad range of values of R_1 and R_v . This implies that the optimum is quite flat and that exact values for R_1 and R_v may not be required. However, this observation is limited to a certain direction in the R_1 - R_v plane. This indicates that one of the degrees of freedom can be left constant, like in the trivial cases. We will follow up on this idea and investigate how the optimal region depends on the feed properties and relative volatilities.

$$V_{opt}(q, z, x_{DA}, x_{BC}, x_{SB}) = \min_{R_1, R_v} V(R_1, R_v, q, z, x_{DA}, x_{BC}, x_{SB})$$

$$(R_1, R_v)_{opt} = f(q, z, x_{DA}, x_{BC}, x_{SB}) \quad (1)$$

3. Computations with an Infinite Number of Stages

We here limit ourselves to sharp splits ($x_{DA} = x_{SB} = x_{BC} = 1$) and an infinite number of stages. Only the main procedure is outlined here; for details, see work by Halvorsen and Skogestad¹⁴ and also Fidkowski and Krolikowski¹⁹ for the minimum reflux computation. We consider a ternary feed mixture with composition $z = [z_A, z_B, z_C]$ for the light, intermediate, and heavy components, respectively. We use a normalized feed ($F = 1$), with liquid fraction q (where $q = 0$ implies a saturated vapor and $q = 1$ implies a saturated liquid). We assume a constant molar overflow and constant relative volatilities $\alpha = [\alpha_A, \alpha_B, \alpha_C]$, referred to a common reference component (usually C). Then we can compute the solution surface $V(R_1, R_v, q, z, \alpha)$. $V(R_1, R_v)$ for a given set of z , q , and α is shown in Figures 2 (surface) and 3 (contour). Note the flat region with $V = V_{min}$ along a straight line from P^* to R^* in the R_1 - R_v plane. This corresponds to the operation along the V-shaped prefractionator minimum reflux characteristics [$L_1 = L_{1,min}(\beta)$], where β is defined as the recovery of the intermediate B component leaving the prefractionator top. The minimum reflux for separating A and C in the prefractionator is denoted the preferred split²⁰ and is obtained with a particular recovery β_P . Point P^* repre-

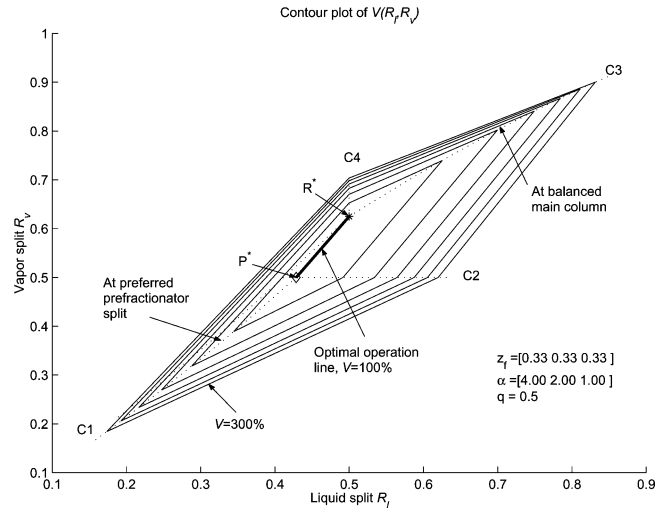


Figure 3. Contour lines for $V(R_1, R_v)$ are straight lines between the four characteristic corners.

sents operation at the preferred split. Point R^* represents the operating point when the top and bottom sections of the main column are both operated at minimum energy. We call this a balanced main column, and the corresponding recovery is β_R . Between P^* and R^* , the minimum energy for the Petlyuk column is constant.

The flat region may be wide or narrow, depending on the relative values of β_P and β_R , and we may have cases with either $\beta_P > \beta_R$ or $\beta_P < \beta_R$ (like in Figures 2 and 3). Only for the special case $\beta_P \approx \beta_R$ do we have a sharp minimum. The mapping between the variables β and L_1 , which is convenient when we look at the prefractionator, and our chosen degrees of freedom R_1 and R_v is straightforward from the definition, and the line segment P^*-R^* is described by the points $(R_{1,P}, R_{v,P})$ in P^* and $(R_{1,R}, R_{v,R})$ in R^* . The minimum boilup rate for the Petlyuk column, which is the boilup when operating along P^*-R^* , is given by

$$V_{min}^{Petlyuk} = \max\left(\frac{\alpha_B z_B}{\theta_A - \alpha_B} + \frac{\alpha_C z_C}{\theta_A - \alpha_C}, \frac{\alpha_C z_C}{\theta_B - \alpha_C}\right) \quad (2)$$

The Underwood roots (θ_A, θ_B) obey $\alpha_A > \theta_A > \alpha_B > \theta_B > \alpha_C$ and can be found by solving eq 3.

$$\frac{\alpha_A z_A}{\alpha_A - \theta} + \frac{\alpha_B z_B}{\alpha_B - \theta} + \frac{\alpha_C z_C}{\alpha_C - \theta} = (1 - q) \quad (3)$$

The minimum vapor flow for the prefractionator for a sharp A/C split is given by

$$V_{1,min}(\beta) = \max\left(\frac{\alpha_A z_A}{\alpha_A - \theta_A} + \frac{\alpha_B z_B \beta}{\alpha_B - \theta_A}, \frac{\alpha_A z_A}{\alpha_A - \theta_B} + \frac{\alpha_B z_B \beta}{\alpha_B - \theta_B}\right) \quad (4)$$

We can find the point of preferred split (β_P) by solving eq 4 for the value of $V_{1,min}$ when both Underwood roots are active [which is at the minimum of the V-shaped $V_{1,min}(\beta)$]. The point of a balanced main column (β_R) can be found by solving the equations for the level lines for the upper and lower parts ($L_{min}^{upper} = L_{min}^{lower}$). These level lines can be expressed as two straight lines in the β - L_1 plane for

the upper and lower parts of the main column:

$$L_1 = L_{\min}^{\text{upper}} - \frac{\beta z_B \alpha_A}{(\alpha_A - \alpha_B) - \frac{z_A \alpha_B}{L_{\min}^{\text{upper}}}} \quad (5)$$

$$L_1 = L_{\min}^{\text{lower}} - z_B - \frac{(1 - \beta) z_B \alpha_C}{(\alpha_B - \alpha_C) - L_{\min}^{\text{lower}} + z_A + z_C - (1 - q)} \quad (6)$$

For nonoptimal operation, away from the line $P^* - R^*$, the details of how to compute an arbitrary point on the solution surface $V(R_i, R_v)$ are given by Halvorsen and Skogestad.¹⁴ A short summary is given here: The contours for $V = \text{constant}$ and $V > V_{\min}$ in the $R_i - R_v$ plane are straight lines between four characteristic corner lines (C1–C4), which represent a particular operating condition for each particular edge (C2 and C4 are for $\beta_P < \beta_R$).

C1: preferred split in the prefractionator; over-refluxed main column.

C2: along the left branch of the minimum reflux characteristics for the prefractionator.

C3: balanced main column and over-refluxed pre-fractionator (above the V-shaped minimum curve).

C4: along the right branch of the minimum reflux characteristics for the prefractionator for $\beta_P > \beta_R$.

The minimum boilup when we fix one of R_i or R_v is along the path C1– $P^* - R^* - C3$: This path is given by $V[R_{i,\text{opt}}(R_v), R_v]$ or $V[R_i, R_{v,\text{opt}}(R_i)]$. Full savings can only be obtained if the chosen constant value is in a flat region (e.g., if $R_{v,p} < R_v < R_{v,R}$), and in addition the other must be optimized for that choice [e.g., $R_i = R_{i,\text{opt}}(R_v)$ when we choose to fix R_v].

4. Results with the Analytical Methods on Some Separation Cases

4.1. When Do We Get the Largest Savings with the Petlyuk Column? The energy savings that can be obtained with a Petlyuk configuration will depend on the feed properties, the product specifications, and the relative volatilities. Our reference for computing the savings is the best of the conventional configuration with direct split (DSL) or indirect split (ISV) (with the vapor feed to the second column). In the triangular plots in Figure 4, we show the contours of the savings as a function of the feed composition (z_A, z_B) for three sets of relative volatilities with a saturated liquid feed.

Observe that the largest savings is obtained for the set of the particular feed compositions when the operating point for a preferred prefractionator split equals the operating point for a balanced main column. This is the situation when P^* coincides with R^* and we have $\beta_P = \beta_R$. This is denoted the “boundary curve” in the following figures. On the side of this boundary closest to the pure C feed, we always have $\beta_P < \beta_R$, and on the side closest to the pure A feed, we always have $\beta_P > \beta_R$. The situation when $P^* = R^*$ is also special when we consider the operational aspects. In that situation, we have no flat region on the solution surface, and this implies that we have to adjust both degrees of freedom online in order to maintain optimal operation for even small feed disturbances. The particular feed composition when we have the largest energy savings will be either at the intersection with the dashed curve where the boilup for

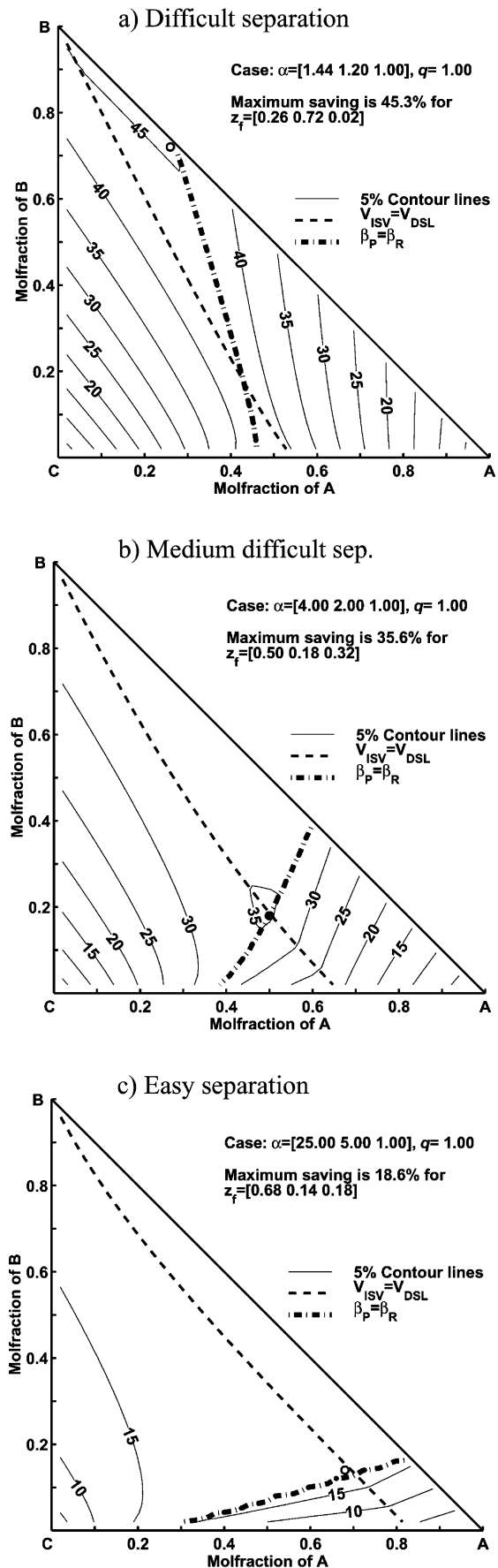


Figure 4. Contour plots of the savings as a function of the feed composition with the Petlyuk column compared to the best of the conventional direct split or indirect split configurations. $\alpha_{AB}/\alpha_{BC} = 1$ for all three cases ($\alpha_{ij} = \alpha_j/\alpha_i$).

the conventional direct split equals the indirect split configuration ($V_{DSL} = V_{ISV}$) or at the end points for the boundary curve for $\beta_P = \beta_R$.

Thus, we get the largest theoretical savings in the region where the column is most difficult to operate optimally and where we also require the largest number of stages.²¹

4.2. Sensitivity to Changes in the Relative Volatility Ratio and Liquid Fraction. The sensitivity of the boundary curve for $\beta_P \approx \beta_R$ to variations in α_{AB}/α_{BC} is very strong as shown for the difficult separation case in Figure 5a,b. In Figure 5c, we observe that changing the feed liquid fraction (q) rotates the boundary curve around an invariant point.

4.3. When Can We Obtain Full Savings with Constant Vapor and Liquid Splits? Assume that the design value for the vapor split has been set to R_v^0 . Figure 6a illustrates the contour lines for constant vapor split values of the end points of P^*R^* , $R_{v,P}$ (solid) and $R_{v,R}$ (dashed), as a function of the feed composition. To be able to operate in the flat optimal region, we must have a feed composition such that $R_{v,P} < R_v^0 < R_{v,R}$ (we always have $R_{v,P} \leq R_{v,R}$).

This is illustrated with the shaded area in Figure 6a for an example with $R_v^0 = 0.6$. Observe that in the feed region close to the boundary curve for $\beta_P = \beta_R$ an operation strategy with constant R_v^0 will only give us full savings for one particular feed composition, but further away from the boundary curve, an exact value of R_v^0 is not required.

The extent of the flat region increases as we move away from the boundary curve. In Figure 6b, $V(R_{l,opt}(R_v), R_v)$ is shown for some selected feed compositions, and we note flat regions.

In Figure 6c, we show an example where we keep both degrees of freedom constant. Now the region where the Petlyuk column savings is positive is even more limited. In Figure 6c, it seems almost impossible to save energy without adjusting R_l and/or R_v to move that narrow region if the feed composition changes.

Let us make a short summary: To operate at minimum energy, we first have to ensure that R_v^0 is in the flat region in order to be within the solution surface $V(R_l, R_v)$ between P^* and R^* at all. This task seems quite easy unless the feed composition is close to the boundary curve. Second, we must find the optimal value of R_l for the particular R_v^0 to ensure that we actually operate on P^*-R^* and not somewhere to the sides of P^*-R^* , where $V(R_l, R_v)$ may be quite steep. With both R_l and R_v constant, the probability of hitting P^*-R^* on a solution surface, which is moved around by changes in z , q , and α , will be very small, so this will only be a feasible strategy if the operating conditions are reasonable steady and for cases where the solution surface is not very steep (which can be the situation for easier separations than for the case in Figure 6c).

5. Simple Procedure To Test the Applicability for a Petlyuk Arrangement

We present a short procedure for evaluating separation cases by the following simple example: We consider the three feed composition regions: I, II, and III, shown in the triangular diagram in Figure 7. The boundary curves for $\beta_P = \beta_R$ (in region X) are computed for the expected variations of the relative volatility and liquid fraction. For feed case I, we have an intersection with

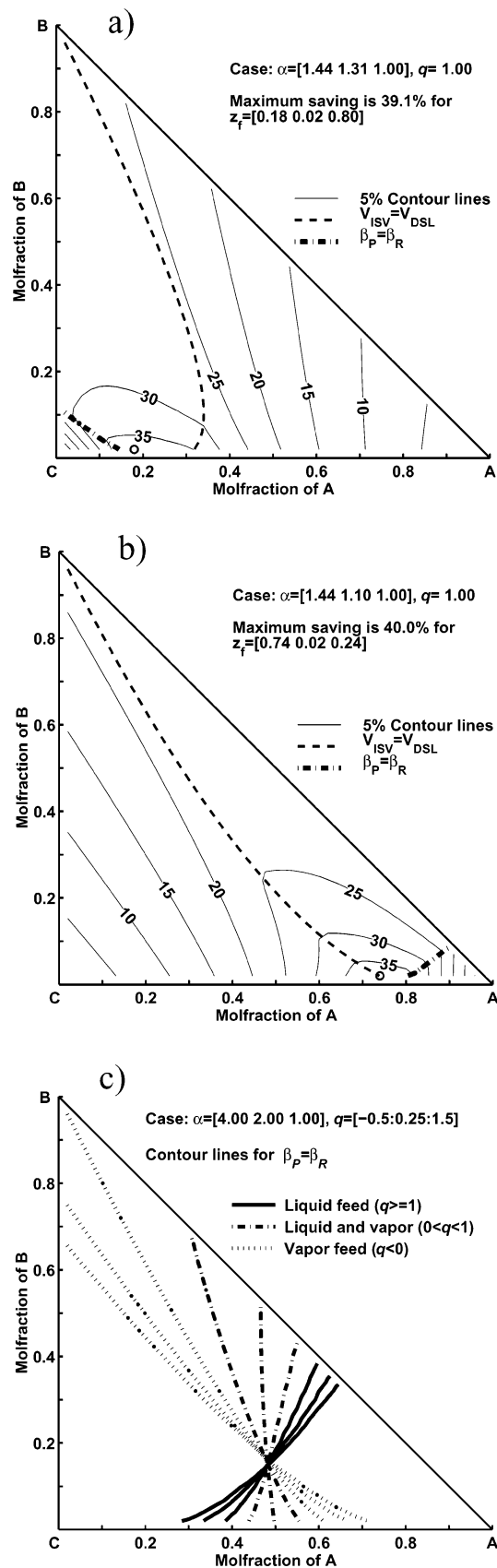


Figure 5. Variation in α_{AB}/α_{BC} , which has a strong impact on the boundary curve for $\beta_P = \beta_R$. The plots show contour lines of the savings with the Petlyuk column compared to the conventional indirect or direct split. The difficulty of the A/C split is the same. (a and b) Difficult case from Figure 4a, here with α_{AB}/α_{BC} set to 1/1.2 and 1.2. (c) Boundary curves for different feed liquid fractions in the range from superheated vapor ($q = -0.5$) in steps of 0.25 to subcooled liquid ($q = -1.5$).

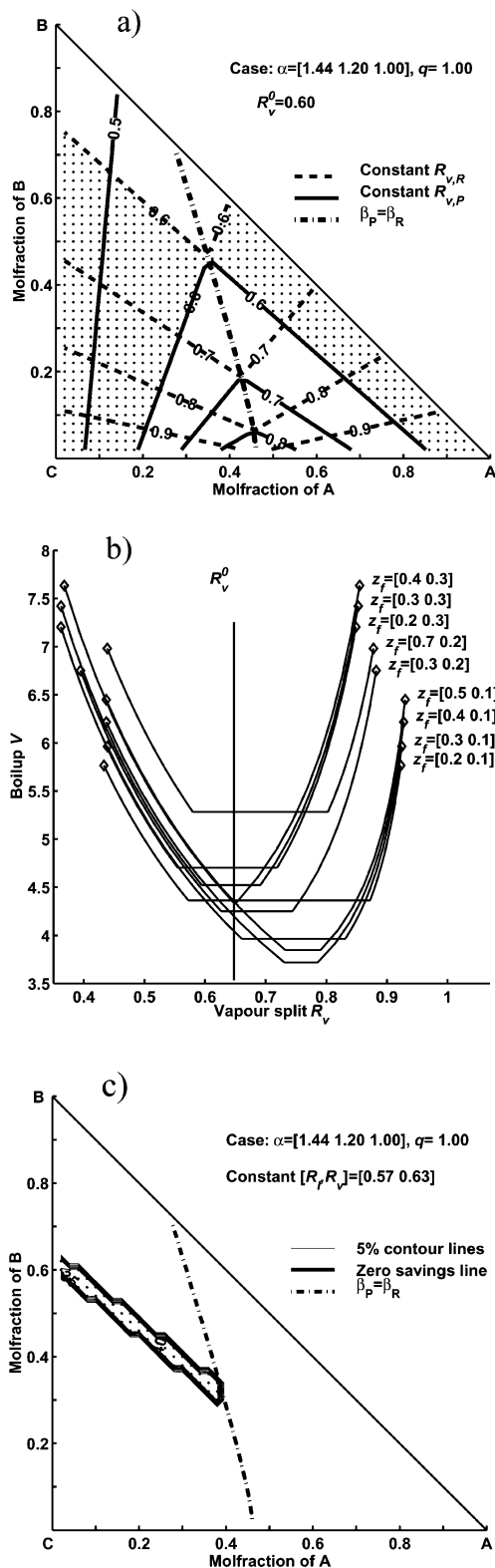


Figure 6. Constant flow splits, which limit energy savings. (a) The contour lines for constant $R_{v,P}$ and $R_{v,R}$ meet at the boundary where for the example with $R_v^0 = 0.6$ full Petlyuk column savings can only be achieved in the shaded region. (b) The plot shows $V[R_{i,opt}(R_v), R_v]$ for some selected feed compositions z_i . These are the path C1–P–R–C3 (see Figures 2 and 3) on each $V(R_i, R_v, z_i)$ that gives the minimum energy as a function of 1 degree of freedom when the other is optimized. (The end-point markers on each curve are at the minimum conventional boilup for each case.) (c) Case where R_i and R_v have been set to the optimal values for $z = (0.33, 0.33, 0.33)$. The narrow shaded area shows the feed composition region where the Petlyuk column performs better than the conventional solution when we fix both R_i and R_v .

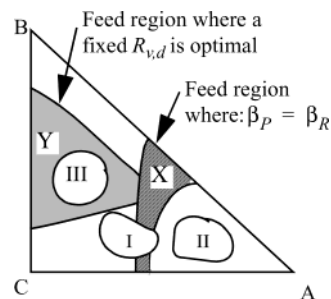


Figure 7. Check the applicability of a Petlyuk arrangement for a given feed property range.

the region X; thus, this case will require online adjustment of both degrees of freedom to achieve the full theoretical energy savings. For cases II and III, we know that there will be a flat region on the solution surface, and the optimal operation will be on the left and right branches of the prefractionator characteristic, respectively. However, if we want to have a fixed vapor split ($R_{v,d}$), the feeds have to be within the region Y in order to get the full benefits of the theoretical energy savings. Thus, only the feed case III will be suitable, for instance, with a DWC with a constant vapor split if we are required to achieve the full theoretical savings of the Petlyuk arrangement. For another value of $R_{v,d}$, region II may also be suitable for operation with a fixed vapor split.

6. Conclusion

Simple analytical Underwood methods developed for the infinite-staged Petlyuk column with a sharp product split can be used to compute the theoretical performance of a Petlyuk arrangement for any set of feed properties and operational situations. For every set of feed parameters and relative volatilities, the full surface $V(R_i, R_v)$ can easily be computed and analyzed. We observe that the best possible energy savings is obtained close to the feed composition region, where the operating point for the preferred split of the prefractionator coincides with the situation that we have the same minimum reflux requirement in the upper and lower parts of the main column, i.e., when the main column is balanced. This region is also the most difficult region for operation because we have to adjust both degrees of freedom online. However, if the feed composition is away from the boundary line, then optimal operation (in terms of minimum boilup) can be obtained with a strategy where one of the degrees of freedom, e.g., the vapor split, is kept constant.

The results shown in this paper are valid for sharp product splits and therefore relevant for high-purity distillation. In the thesis by Halvorsen²¹ (Chapter 9), the case of nonsharp splits, including new analytical expressions for the infinite-staged case, is treated further, and it is shown that, in particular, the side-stream purity is closely related to the extent of the flat region of $V(R_i, R_v)$. A typical symptom of a real column if we have a feed composition outside the feasible regions for high-purity operation is that we will be unable to produce high-purity products, even if the energy input to the column is above the theoretical minimum. So, instead of an increase in the energy consumption for nonoptimal operation, we may experience a decreasing product purity, particularly in the side stream.

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