Use of Short-cut Methods to Analyse Optimal Operation of Petlyuk Distillation Columns

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Abstract:

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

Keywords: Petlyuk distillation column, dividing wall column, optimizing control, minimum energy

1. INTRODUCTION

The fully thermally coupled distillation arrangement, (Petlyuk 1965), has several appealing features for separation of a three-component mixture. However, the industrial usage have been quite limited, although it is 50 years since the patent of (Wright 1949) for a dividing wall column. The sole industrial exception has been BASF, e.g. (Kaibel 1997), which have several dividing wall columns in operation and regard it as standard technology. Recently, a Japanese and a British application have been reported, (Parkinson 1998) and (Lestak et al. 1999). Theoretical design studies, and results from pilot plant operation have been presented by (Triantafyllou and Smith 1992) and (Mutalib and Smith 1998). Recent theoretical studies are presented by (Mizsey et. al. 1998) and (Agrawal and Fidkowski 1998a,b). All authors report typical savings in the order of 30% in energy costs, and 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 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 to the design of number of stages in each column section.

2. THE PETLYUK DISTILLATION COLUMN

The Petlyuk column, shown in figure 1, has at steady state five degrees of freedom, which may be selected as the following manipulated input variables: Boilup (*V*), reflux (*L*), mid product side-stream flow (*S*), liquid split $(R_l = L_l/L)$ and vapour split $(R_v = V_2/V)$. There are three main product purity specifications: Top (x_{Da}) , bottoms (x_{Bc}) and side-stream (x_{Sb}) . A very important issue is then that we have more degrees of freedom (5) than product specifications (3 in this example). The two extra degrees of freedom can be used for optimization purposes, like minimization of the energy consumption. When the column is operated optimally, the infinite staged Petlyuk column always consumes less energy than the corresponding conventional solution, (Fidkowski 1987). However, this optimal operation may be difficult to achieve in practice since the optimal operation depends strongly on the feed properties and the remaining degrees of freedom.(Wolff and Skogestad 1994) and (Halvorsen and Skogestad 1999a).

In the following we will choose L,V and S to control the product purities, and let (R_l, R_v) be the remaining two 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, R_v) , the feed properties (z, q) and the product specifications (x_{Da}, x_{Bo}, x_{Sb}) . We choose to use the reboiler vapour 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 boilup (V_{opt}) will be a function of feed properties and product specifications, but not the degrees of freedom. The optimal values R_l and R_v can be found by minimizing the boilup with respect to the degrees of freedom as shown in equation (1).

An important observation for the Petlyuk column is that $V \approx V_{opt}$ for a broad range of values of (R_l, R_v) . This implies that the optimum is quite flat and that exact values for (R_l, R_v) may not be required. However, this observation is limited to a certain direction in the (R_l, 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 this idea and investigate how the optimal region depend on the feed properties and relative volatilities.

$$
V_{opt}(q, z, x_{Da}, x_{Bc}, x_{Sb}) = \min_{(R_b, R_v)} V(R_b, R_v, q, z, x_{Da}, x_{Bc}, x_{Sb})
$$

$$
(R_b, R_v)_{opt} = f(q, z, x_{Da}, x_{Bc}, x_{Sb})
$$
 (1)

3. COMPUTATIONS WITH INFINITE NUMBER OF STAGES

We here limit ourselves to sharp splits ($x_{Da} = x_{Bc} = x_{Sb} = 1$) and infinite number of stages. Only the main procedure is outlined here; for details see (Halvorsen and Skogestad 1999a,b) and also (Fidkowski 1986) for the minimum reflux computation. We assume a ternary feed mixture with composition $z = [z_A, z_B, z_C]$ for the light, intermediate and heavy components respectively. We use normalized feed $(F=1)$, with liquid fraction *q* (where *q*=0 implies saturated vapour and *q*=1 implies saturated liquid). We assume 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 $V(R_l, R_v, q, z, \alpha)$. $V(R_h, R_v)$ for a given set of *z,q* and α is shown in figure 2 (surface) and 3 (contour). Note the flat region

with infinite stages and sharp splits

Figure 2: The solution surface $V(R_hR_v)$ for the case Figure 3: The contour lines for $V(R_hR_v)$ are straight lines between the four characteristic corners

with $V=V_{min}$ along a straight line from P^* to R^* in the (R_i, R_y) -plane. This corresponds to the operation along the V-shaped prefractionator minimum reflux characteristics ($L_1 = L_1_{min}(\beta)$). between the point of the preferred split (β_p) in P^{*}, and the value (β_g) which makes the main column balanced in R^{*}. β is defined as the recovery of the intermediate B-component leaving the prefractionator top. $L_I = L_{I, min}(\beta)$ $β_P$) in P^{*}, and the value ($β_R$) which makes the main column balanced in R^{*}. β

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 figure 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, L_1) , which are convenient when we look at the prefractionator, and our chosen degrees of freedom (R_l, R_v) is straightforward from the definition, and the line segment P*R* is described by the points $(R_{l, P}, R_{v, P})$ in P* and $(R_{l, R}, R_{v, R})$ in R*. The minimum boilup rate for the Petlyuk column, which is the boilup when operating along \tilde{P}^*R^* , is given by:

$$
V_{min}^{petlyuk} = max \left(\frac{\alpha_B z_B}{\phi_I - \alpha_B} + \frac{\alpha_C z_C}{\phi_I - \alpha_C}, \frac{\alpha_C z_C}{\phi_2 - \alpha_C} \right)
$$
(2)

The Underwood roots (ϕ_1, ϕ_2) obey $\alpha_A > \phi_1 > \alpha_B > \phi_2 > \alpha_C$ and can be found by solving equation (3):

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

The minimum vapour flow for the prefractionator for sharp A/C split is then given by:

$$
V_{I, min}(\beta) = \frac{max}{\phi_I, \phi_2} \left(\frac{\alpha_A z_A}{\alpha_A - \phi} + \frac{\alpha_B z_B \beta}{\alpha_B - \phi} \right)
$$
(4)

We can find the point of preferred split (β_P) by solving (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 same minimum main column reflux for the upper an lower part ($L_{min}^{upper} = L_{min}^{lower}$). These level lines can be expressed as two straight lines in the (β, L_1) -plane for the upper and lower part of the main column: $L_{min}^{upper} = L_{min}^{lower}$ β, *L1*

$$
L_{I} = L_{min}^{upper} - \frac{\beta z_{B}\alpha_{A}}{(\alpha_{A} - \alpha_{B}) - \frac{z_{A}a_{B}}{L_{min}^{upper}}} \qquad L_{I} = L_{min}^{lower} - z_{B} - \frac{(1 - \beta)z_{B}\alpha_{C}}{(\alpha_{B} - \alpha_{C}) - \frac{z_{C}a_{B}}{L_{min}^{lower} + z_{A} + z_{C} - (1 - q)}}
$$
(5)

For non-optimal operation, away from the line P^*R^* , the details of how to compute an arbitrary point on the solution surface $V(R_h, R_v)$ is given in (Halvorsen and Skogestad 1999a,b). A short summary is given here: The contours for $(V=const, V>V_{min})$ in the (R_l, 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 prefractionator (above the V-shaped minimum curve).
- C4: Along the right branch of the minimum reflux characteristics for the prefractionator for $\beta > \beta_R$

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

4. RESULTS WITH THE ANALYTICAL METHODS FOR 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 vapour 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 saturated liquid feed.

Observe that the largest saving 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 pure C-feed we always have $\beta_P < \beta_R$, and on the side most close to 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 on-line 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 the conventional direct split equals the indirect split configuration, $(V_{DSL} = V_{ISV})$ or at the end-points for the boundary curve for $\beta_P = \beta_R$.

Figure 4: Contour plots of the savings as function of 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 $(\alpha_{ij} = \alpha_i/\alpha_j)$.

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, see (Halvorsen and Skogestad 1999b).

4.2 Sensitivity to changes in relative volatility ratio (α_{AB}/α_{BC}) and liquid fraction (q)

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 and 5b. In figure 5c we observe that changing the feed liquid fraction (*q*) rotates the boundary curve around an invariant point.

Figure 5: Variation in α_{AB}/α_{BC} has 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 as in figure 4.

- a) and b) show the difficult case from figure 4a), here with α_{AB}/α_{BC} set to 1/1.2 and 1.2.
- c) The plots show boundary curves for different the feed liquid fractions in the range from from superheated vapour $(q=0.5)$ in steps of 0.25 through to sub-cooled liquid $(q=1.5)$.

4.3 When can we obtain full savings with constant vapour and liquid splits?

Assume that the design value for the vapour split has been set to $R_v^{\hat{o}}$. Figure 6a illustrates the contour lines for constant vapour split values of the end-points of P^*R^* , $R_{v,P}$ (solid) and $R_{v,R}$ (dashed) as a function of feed composition. In order to be able to operate in the flat optimal region, we must have a feed composition such that R_{v} , R_{v} $\lt R_{v}$, R_{v} . (We have always: R_{v} , R_{v} , R_{v}). 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 , an operation strategy with constant R_v^{\prime} will only give us full savings for one particular feed composition, but further away from the boundary curve, an exact value of R_v^{\prime} is not required. $R_{v, p} < R_v^o < R_{v, R}$. (We have always: $R_{v, p} \le R_{v, R}$ R_v^o $β_P = β_R$, an operation strategy with constant R^o_v *o*

Figure 6:a) The contour lines for constant $R_{v,P}$ and $R_{v,R}$ meet at the boundary where $\beta_P = \beta_R$. For the example with R_v^0 =0.6, full Petlyuk column savings can only be achieved in the shaded region. b) The plot show $V(R_{l,opt}(R_v), R_v)$ for some selected feed compositions z_i . These are the path C1-P-R-C3 (see figure 2 and 3) on each $V(R_l, R_v, z_i)$ which gives the minimum energy as function of one degree of freedom when the other is optimized. (The endpoint markers on each curve are at the minimum conventional boilup for each case.)

c) Case where R_l and R_v have been set to the optimal values for $z=[0.33,0.33,0.33]$. The narrow shaded area show the feed composition region where the Petlyuk column perform better than the conventional solution when we fix both R_l and R_v .

The extent of the flat region increase 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 wee keep *both* degrees of freedom constant. Now the region where 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^o is in the flat region in order be able to hit the solution surface $V(R_l, R_v)$ between P^{*} and R^{*} at all. This task seem quite easy unless when 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 fig. 6c).

5. A SIMPLE PROCEDURE TO TEST THE APPLICABILITY FOR A PETLYUK ARRANGEMENT

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

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 relative volatility and liquid fraction. For feed case I, we have an intersection with the region X, thus this case will require on-line adjustment of both degrees of freedom to achieve the full theoretical energy saving. For case 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 branch of the prefractionator characteristic, respectively. However, if we want to have a fixed vapour split $(R_{v,d})$, the feed have to be within the region Y in order to get the full benefits of the theoretical energy saving. Thus only the feed case III will be suitable for instance with a DWC with the constant vapour 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 vapour split.

6. CONCLUSION

Simple analytical Underwood methods developed for the infinite staged Petlyuk column with 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 $V(R_l, R_v)$ can easily be computed and analysed. We observe that the best possible energy savings is obtained close to the feed composition region where the operating point for preferred split of the prefractionator coincide with the situation that we have the same minimum reflux requirement in the upper and lower part of the main column, i.e when the main column is balanced. This region is also the most difficult region for operation since we have to adjust both degrees of freedom on-line. 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 vapour split, is kept constant.

The results shown in this paper are valid for sharp product splits, and therefore relevant for high purity distillation. In (Halvorsen and Skogestad 1999b) the case of non-sharp splits, including new analytical expressions for the infinite stage case, is treated further and it is shown that in particular the sidestream purity is closely related to the extent of the flat region of $V(R_hR_v)$. A typical symptom on 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 increase in energy consumption for non-optimal operation, we may experience a decreasing product purity.

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