Optimizing Control of Petlyuk Distillation: Understanding the Steady-State Behavior

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Abstract.

The "Petlyuk" or "dividing-wall" or "fully thermally coupled" distillation column is an interesting alternative to the conventional cascaded binary columns for separation of multi-component mixtures. The industrial use has been very limited, and difficulties in control has been reported as one reason. Since we have more manipulated variables than controlled variables, the column is a candidate for on-line optimization. We show that the steady-state optimal solution surface is quite narrow, and depend strongly on disturbances and design parameters. Thus it seems difficult to achieve the potential energy savings compared to traditional approaches without a good control strategy.

1. INTRODUCTION

The thermally integrated "Petlyuk" arrangement implemented in a single distillation column shell has several appealing features. For the separation of a three-component mixture, *Triantafyllou and Smith (1992)* report savings in the order of 30% in both capital and energy costs compared to traditional arrangements with binary columns in series.

An important question remains: Is this process units difficult to operate and is it possible to achieve in practice the energy savings?

The Petlyuk column, shown in Fig. 1, has at steady state, five independent manipulated inputs: Boilup (V), reflux (L), mid product side-stream flow (S), liquid split (R_l) and vapor split (R_v). There may be up to four product specifications: Purities of top (x_{Da}) and bottom (x_{Bc}) products, purity of side-stream product (x_{Sb})and the ratio of the light and heavy impurity components in the side-stream product (x_{Sa}/x_{Sc}).

However, *Wolff, Skogestad and Havre (1994)* have reported discontinuities in the range of feasible operation if all these four product compositions are specified. This is related to the fact that column sections 4 and 5 (see Fig. 1) are tightly coupled and we cannot independently adjust the amount of light and heavy component in the side stream. On the other hand, if the number of controlled outputs is reduced from four to three, by not considering the ratio of light/heavy impurity-components in the side-stream, the feasibility problem disappears. In this paper we will focus on this simpler task of three-point control. Due to the fact that we have more manipulative inputs than controlled compositions, the remaining two manipulative variables can be used for other purposes, and in particular for minimizing the operating cost.

Three main classes of methods for solving this kind of optimization problem can be mentioned: Model based methods, experimenting methods (e.g. EVOP) and feedback methods. Note that standard linear model predictive control methods (MPC), do not handle this kind of nonlinear optimization problem, but rather a multivariable

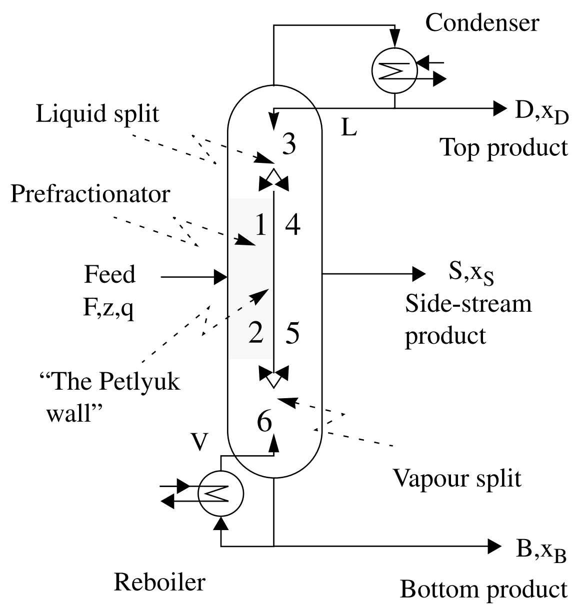

Fig. 1 The Petlyuk Distillation Column

setpoint control problem with constraints. However, nonlinear model based methods may be applicable. The problems of model uncertainty and unknown disturbances may be overcome by good estimation techniques. Nonlinear MPC is certainly a candidate for future applications.

In this paper we will focus on the feedback method. This is the simplest method, requiring the least modeling effort for implementation, and is therefore the preferred choice if it gives acceptable performance. For the Petlyuk column studied in this paper the optimization objective is to use the two extra manipulated inputs (e.g. R_l and R_v) to minimize the energy consumption (V/F). The key idea for the feedback method is to translate this optimization problem into a setpoint problem.

The issue is then to find a set of variables which, when kept constant at their setpoints, indirectly ensures optimal operation. A simple daily life example is the process of baking an "optimal cake", which is a very difficult modeling and optimization problem. However, we know that almost optimal operation is obtained when we use feed-

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back control where the oven temperature is kept at a given setpoint, e.g. 200 °C. Another example is a conventional distillation column where the product compositions are often set as an indirect way of minimizing the overall operational cost, and not because the compositions are specified.

To return to the Petlyuk column, one seemingly viable solution would be to simply implement the optimal minimum heat input in an open loop fashion (i. e. set $V = V_{min}$). However, there are at least three serious problems: 1) Since operation is infeasible if we have $V < V_{min}$, we would need to set $V > V_{min}$. 2) Measurement or estimation of the actual V is generally difficult and inaccurate, which makes it even more difficult to keep V close to V_{min}. 3) The optimal value V_{min} changes with operation, and it would require a good model and measurements of the disturbances to recompute it.

Thus, this open-loop policy is clearly not viable. As good candidate variables for feedback control we want variables which avoid the three problems above: 1) The optimal candidate feedback value should not be at a limit. 2) The variable should not have an extremum inside the normal operating range, and in particular not when $V = V_{min}$ 3) The accuracy of the measurement of the variable should be good. 4) The relation of the variable and the optimum should be insensitive to disturbances. 5) Finally, the variable should be easy to control, using the available extra degrees of freedom.

Often we may find variables which have an extremum when the criterion functions is at its minimum. These cannot be used for feedback, but may be used in experimental methods, or simply as indicators to process operators.

A variable related to the gradient of the criterion function will fulfill the most important requirements, and can be used for feedback.

In general it is not always possible to find a feedback variable with the required property of turning the optimization problem into a setpoint problem. However, for processes with a large number of states, and a large number of ways to combine measurements, good candidates may exist, but they may not be straightforward to find.

Skogestad and Postlethwaite (1996) present a method for selecting the best candidate feedback variables from a set of available alternatives. We will not consider this procedure here, but rather aim at obtaining insight into the column behavior which may be used for selecting candidate feedback variables.

2. THE PETLYUK COLUMN MODEL

We use a dynamic tray model with the following simplifying assumptions: Constant pressure, constant relative volatilities, constant molar flows, constant tray efficiency, no heat transfer through the dividing wall. This is a very simple model, but it contains the most important properties of a column. The column data are given in appendix A-3.

The column shown in Fig. 1 is modeled with 6 sections (the numbers inside the column are section numbers). A three-component feed, with components *a, b* and *c* is separated into almost pure *a* (97%) in the top product D, almost pure *b* (97%) in the in the side stream S, and almost pure *c* (97%) in the bottom product B. The overall model can be represented on a general state space form:

$$\begin{aligned} d\frac{x(t)}{dt} &= f(x(t), u(t), d(t)) \\ y(t) &= g(x(t), u(t)) \end{aligned} \tag{1}$$

The states x(t) consist of the component holdups on each tray, that is three states for each tray, which we represent using two compositions and the total holdup. For our column, as described in appendix A-3 the total number of states is 150 (48 trays plus reboiler and condenser). Note that the steady state composition profile does not depend on tray hydraulics nor on the accumulator dynamics. However, the flow and accumulator dynamics will have an impact on the high frequency properties of the column, and may play an important role in controller design.

The input, output and disturbance vectors are defined as:

$$\begin{aligned} u &= [L, V, S, R_l, R_v] \\ y &= [x_{Da}, x_{Bc}, x_{Sb}] \\ d &= [F, z_a, z_b, q] \end{aligned} \tag{2}$$

In addition to the y-vector described here, we will propose later some other measurements to be used for optimization purposes.

3. STEADY-STATE SOLUTION

3.1 Optimization Criterion

With 5 control inputs and 3 setpoints specified we have left 2 degrees-of-freedom for optimization. We here choose the two remaining degrees-of-freedom to be R_l and R_v, but note that other choices may be made.

A comprehensive optimization criterion should include product values and energy cost and be based om maximizing the operational profit. But if we specify product purities, then a very suitable criterion, selected here, is to minimize the energy consumption. In this paper, we use boilup rate (V) as the criterion value, and this will be equivalent to use the energy consumption for most columns.

The steady state constrained optimization problem can be written on the following general form:

$$\min_{u} \quad V(x, u, d) \tag{3}$$

$$\begin{aligned} \frac{dx}{dt} &= f(x, u, d) = 0 \\ h(x, u) &\le 0 \end{aligned} \tag{4}$$

The first set of equality constraints represents the steady state model, the second set of equality or inequality constraints will typically contain product specifications (e.g. $x_{Da} > 0.97$) and also allowed range for u (e.g $u_{min} \le u \le u_{max}$).

3.2 Steady State Profiles

We here consider the optimal steady state solution with three specified compositions and with the two remaining degrees-of-freedom (R_l,R_v) chosen such that the vapor boilup V (energy consumption) is minimized.

Fig. 2 shows the resulting composition profile. We observe that the prefractionator separates *a* from *c* almost

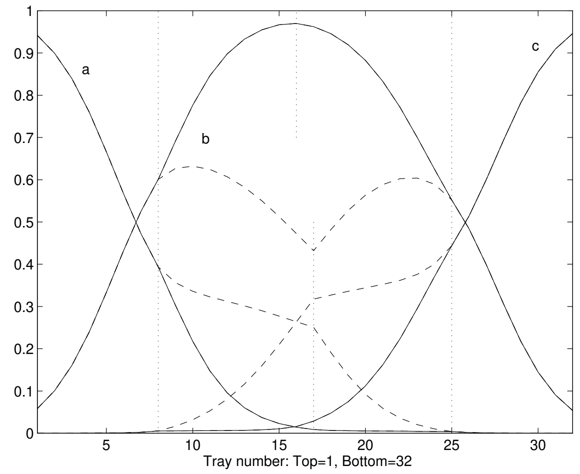

Fig. 2 Compositions of components *a, b* and *c* in prefractionator (dashed) and main column (solid).

completely. Thus we can regard sections 3+4 as a binary column for separation of *a* and *b*, and sections 5+6 as a binary column for separation of *b* and *c*. The "tricky" part is that the "feed" to 3+4 and 5+6 depends on the control inputs *u*, and that we have the same vapor flow in sections 5 and 4. We observe that the tray with maximum b-composition is the side-stream tray, which intuitively seems reasonable.

Normally, composition measurements along the column are not available, but temperatures, which are closely related to compositions, may be used to obtain important information. A simple temperature model is used here: We just assume that the temperature on a tray (i) is the mole fraction average of the boiling points T_B for each components (j):

$$T_i = \sum_{j = a, b, c} T_{Bj} x_{i, j} \tag{5}$$

In Fig. 3, the three boiling points are set to [0,50,100] for light, medium and heavy component, respectively.

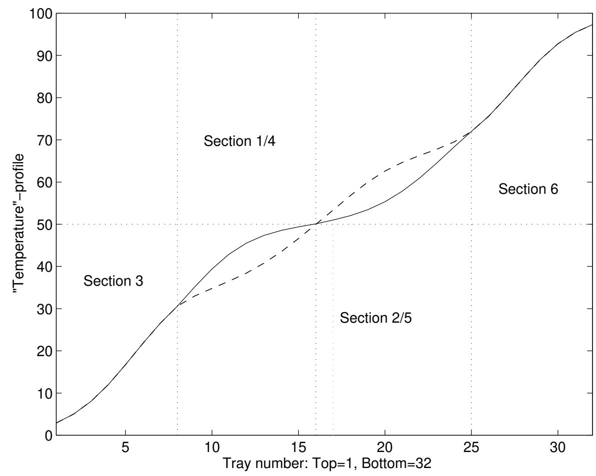

Fig. 3 Temperature profile in prefractionator (dashed) and main column (solid)

At the product locations, the temperature profile is close to the pure product boiling point, and the temperature profile will normally have large gradients where the composition profile has large gradients.

3.3 The solution surface

We now want to study the sensitivity of the optimal solution to variations in R_l and R_v. The solution of the model equations (4), with R_l and R_v as parameters, can be written as:

$$V = J(R_l, R_v) \tag{6}$$

The solution surface is shown in Fig. 4 and Fig. 5 for the "symmetric" case where the feed is 50% vapor (q=0.5). It actually looks like a hull of a ship. The minimum vapor flow is $V_{min} \approx 1.5$, but observe that the vapor flow increase rapidly if we do not keep [R_l,R_v] on their optimal values [0.45 0.49]. In the "worst" direction, which is from the optimum towards P (P is hidden in Fig. 4) or Q, the boilup increase by 50% for a change in R_l or R_v of just 1%. In the "best" direction, which is towards Z or X, R_l *or* R_v can be changed by 0.25 or 50% before the boilup increases by 50%.

The conclusion of this is that at least one of the remaining degrees-of-freedom (R_l *or* R_v) have to be manipulated by some control algorithm in order to achieve close to optimal operation. But is seems possible that one, for instance R_v can kept constant, but then R_l has to be adjusted to keep the operating point in the bottom of the valley between Z and X.

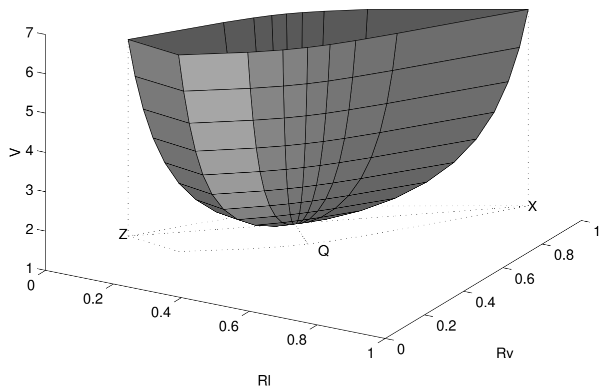

Fig. 4 Optimal solution surface. $V=J(R_l,R_v)$. q=0.5

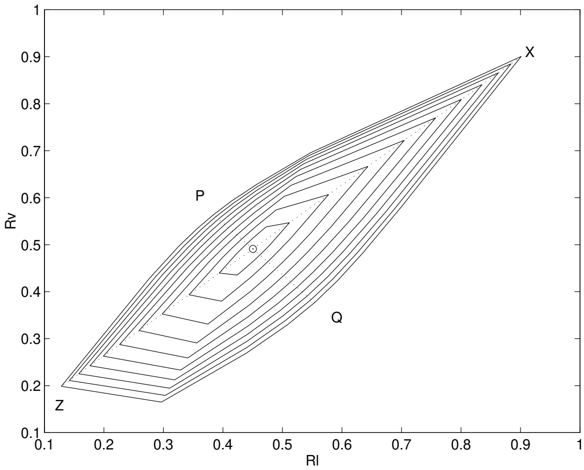

Fig. 5 Contour plot of $V=J(R_l,R_v)$. q=0.5 (Note that the change in boilup between contour lines is not constant, but quadratic)

3.4 Effect of disturbances

If disturbances or setpoint changes move the optimum in the PQ direction, then this results in large increases in V unless we adjust R_l *or* R_v in order to remain in the "bottom of the valley". Fig. 6 show how the optimal values of R_l

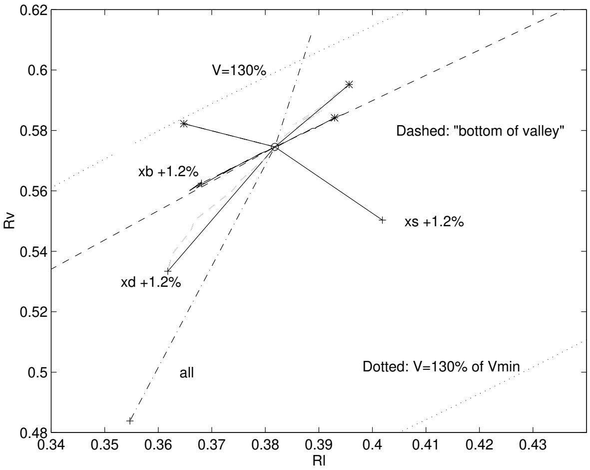

Fig. 6 Effect on optimal $[R_l,R_v]$ from setpoint changes in product purity (96%-98.2%, 97% in the "centre").

and R_v are affected by individual changes in the product compositions. On the figure we also show the "bottom of the valley" (dashed) as well as lines with constant boilup at 30% above optimum (dotted). Observe that changes in bottom product composition move the optimum along the valley (in XZ direction), whereas changes to the side-stream composition move the optimum in the "worst" direction (along PQ). If the feed composition is changed (not shown in any figure), we will get the largest effect along the valley, but the direction will depend on how feed composition is changed. Changing the feed enthalpy (q) moves optimum in the PQ direction. In addition, as shown in Fig. 7, changes in the feed enthalpy have a dramatic

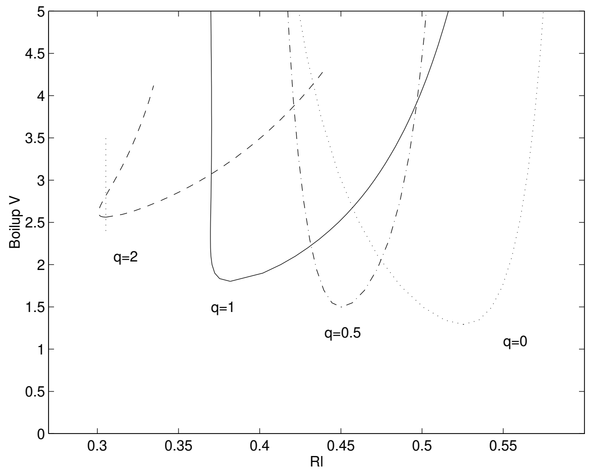

Fig. 7 Solution surface dependence of feed enthalpy factor. Projection into vertical plane through PQ.

effect on the shape of the solution surface. When the feed is saturated liquid (q=1), the optimal surface becomes almost vertical very close to the optimum. The practical implication of this is that with R_l and R_v fixed at a point close to the optimum, the system may easily become unstable, since no amount of energy can fulfill the composition requirements. For subcooled liquid, the solution surface in P direction "bends" over towards Q, and we may have multiple solutions of V for the same product compositions. In open loop, all these operation conditions are reachable and stable. But with composition control active, and tuned for the lower branch, operation on the upper branch is unstable (see curve for q= 2).

Feed flow rate change will not affect the steady state values of optimal split ratios. But feed flow rate upsets are normally a major disturbance and will affect the composition control and optimization during a transient.

3.5 Net Component Flow

Interesting insights into the behavior of the column are obtained by considering the transport of each component in the feed, through the column section and to the products. Define the *net upwards component flow* in a section as:

$$w_j = V_i y_{i,j} - L_{i+1} x_{i+1,j} \tag{7}$$

At steady state this is a constant through each section. By analyzing w_j for the optimal solution we observe that the component flows are as indicated in Fig. 8. For example

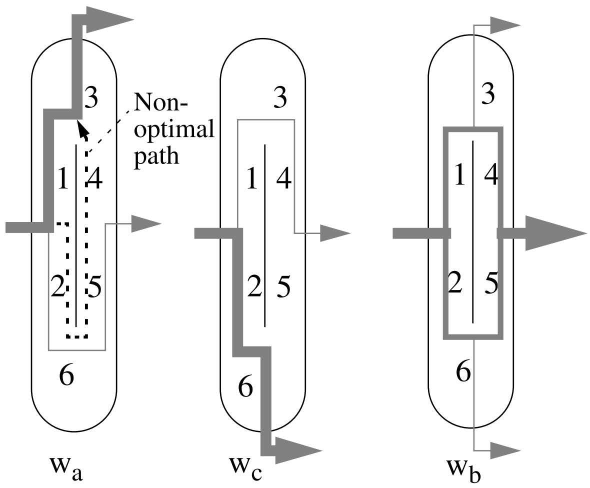

Fig. 8 Components taking "shortest" way through

if we look at the light a-component, then most of the flow take the "shortest" way out to the top product. Some light product "slips" down the prefractionator and this ends up in the side stream. Interestingly, for the optimal solution there is no net flow of light component in the section above the side stream, that is, w_{a4} is close to zero. (We know that $w_{a4} > 0$ is bad, but we might have expected that some of the light component should travel downwards in section 4.) For the heavy component (c) the picture is similar, but reversed.

4. CANDIDATE FEEDBACK VARIABLES

The results above show that we must at least adjust one of the remaining degrees-of-freedom if close to optimal operation is desired. As mentioned in the introduction, we would like to find some feedback measurement, which when kept constant, would ensure optimal operation.

Candidates for such measurements are composition measurements on individual trays, temperature measurements, and combinations of temperature measurements, and we may also consider flow measurements from individual sections of the column. Temperatures are easy to measure, flows are more difficult, and so are also compositions.

4.1 Net total material flow

Consider the net total material flows in the sections, in particular above and below the side-stream. As mentioned earlier, sections 3+4 and sections 5+6 can be regarded as two binary columns. Let us define the net flow downwards in section 4 and upwards in section 5 as B_4 and D_5 respectively.

$$B_4 = L_4 - V_4 \qquad D_5 = V_5 - L_5 \tag{8}$$

These must satisfy: $S=B_4+D_5$, and we would expect that B_4 and D_5 should both be positive. This insight is correct, as we find in non-optimal operating points that B_4 or D_5 may be negative. This is illustrated for B_4 in Fig. 9, where

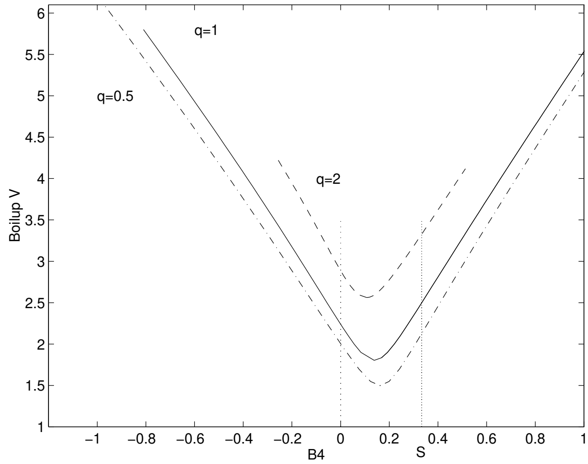

Fig. 9 Boilup as function of net downwards flow above the side stream (B_4) in the "bad" PQ direction of the solution surface (recall Fig. 4).

we see that B_4 changes almost proportionally to the boilup when we move along the solution surface in the PQ direction. Note that optimum value of B_4 is close to *S/2,* and that this value is quite insensitive to the feed enthalpy (q). In the bottom of the V-surface valley, (ZX-direction), the values of B_4 and D_5 are also approximately constant and close to S/2. Thus if we were able to measure the net flow B_4 or D_5, then we could achieve close to optimal operation by adjusting R_l to keep $B_4 = S/2$. Unfortunately such a flow measurement is difficult to obtain in practice.

4.2 Position of Profile in Main Column.

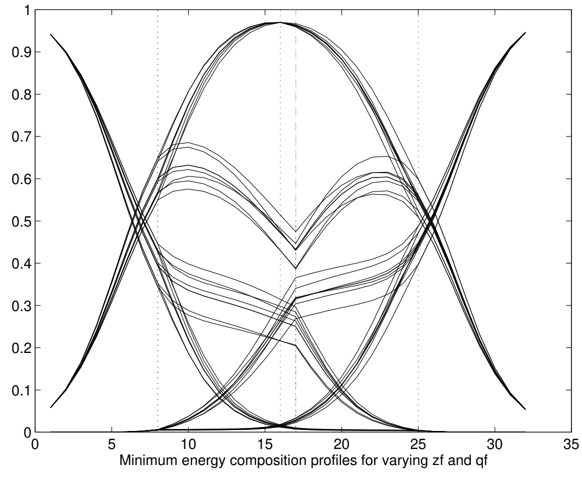

Fig. 10 Composition profiles for varying disturbances

Another important observation is that the maximum composition of the mid-component occurs at the side-stream tray when the column is at its optimum (Fig. 10). This is also approximately true along the bottom of the surface valley. Detecting the actual stage with the maximum value of x_b could thus be a perfect candidate for feedback optimization. However, it is difficult to measure and it also seems to be rather insensitive, so it might be difficult to use in practice

4.3 Temperature Profile Symmetry

Some interesting observations have been made by looking at the symmetry properties of the temperature profile. We define the signed value of the area between the temperature profiles on each side of the dividing wall as a symmetry measurement (DT_S). In a practical application DT_S can be based on or more pairs of difference temperatures in sections above and below feed and side stream.

$$DT_S = \sum (T_{1,i} - T_{4,i}) + \sum (T_{2,i} - T_{5,i}) \tag{9}$$

The profile in Fig. 3 represents an optimum. Fig. 11 shows the profiles if we move away from the optimum in the four directions towards P,X,Z and Q of Fig. 4. (Note that q=1 in figures 3 and 11.) Interestingly we find DT_S close to zero (symmetric profiles) not only around the optimum, but also along the whole "bottom of the valley" of the solution surface. (between X and Z in Fig. 4). When

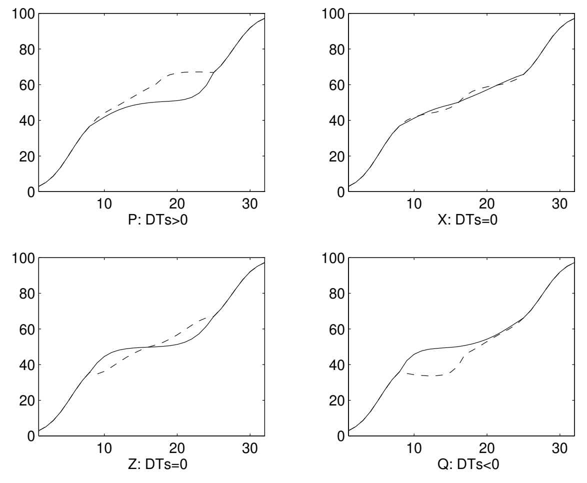

Fig. 11 Temperature profiles for off-optimal operation in directions along the bottom valley (ZX) and in the bad direction perpendicular to the valley (PQ).

we move away from the bottom of the valley in PQ-direction, the profile symmetry changes, and the symmetry measure DT_S increases towards P and it decreases towards Q. In Fig. 12 it is shown that if we keep DT_S=k, where k is a constant, this corresponds to an operating line parallel to the bottom of the valley.Unfortunately, the optimal value of DT_S is also sensitive to disturbances, but it may still give important information. DT_s is easy to measure. A practical operating strategy may be to fix R_v, and control the remaining 4x4 system with $[L,V,S,R_l]$ as inputs and $[x_{Da},x_{Bc},x_{Sb},DT_S]$ as measurements. By selecting a suitable setpoint for DT_S we will keep the operating point at a line parallel to the bottom of the optimal surface valley. We may possibly correct the value of DT_S by observing the location of maximum x_b in the main column (see 4.2).

5. VARIABLES RELATED TO THE CRITERION

Some other variables which have an extremal value when $V = V_{min}$ can also be found. These values can not be

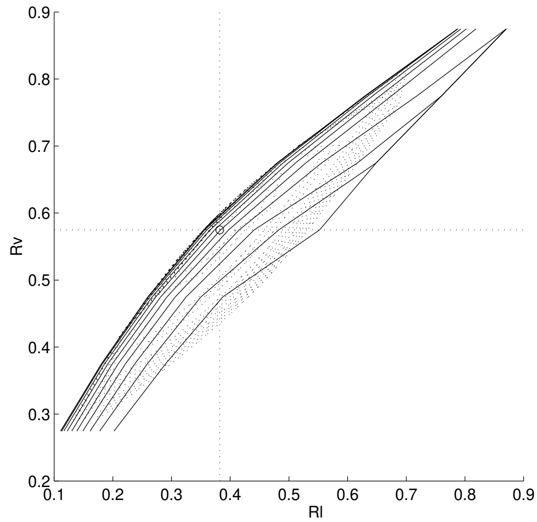

Fig. 12 Operating lines R_l=$f(R_v)$ when DT_s=k for some values of k. Contour lines for constant V is shown dotted. (Feed is saturated liquid, q=1)

used as feedback for setpoint control close to optimum, but may be used as a direct indicator of the criterion value, and for example, in an on-line experimenting method.

One such value is *the temperature difference over the pre-fractionator*. We observe that the temperature difference over the pre-fractionator always has its maximum when the boilup is at its minimum. This temperature difference is related to properties of the composition profile through the simple temperature model in equation (5), so it really reflects optimal separation over the column sections on each side of the dividing wall.

6. CONCLUSIONS

The Petlyuk distillation column will most likely require some kind of optimizing control in order to realize its full potential for reduced energy consumption. This is because the solution surface of the criterion function is quite narrow, and the operation is very sensitive to certain disturbances. In this paper we have obtained some relationships between optimal operation and some measurements which can be deduced from the composition profile or the states. This may be used to select candidate feedback variables. Optimization by feedback should be compared to nonlinear model-based optimization methods, and evaluated for complexity and performance.

7. ACKNOWLEDGEMENTS

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Appendix A

A.1 Model equations

The model equations are quite standard and are described below. Component mass balance on a tray i is given by (component indices on x and y are omitted):

$$M_i\frac{dx_i}{dt} = L_{i+1}(x_{i+1}-x_i)+V_{i-1}(y_{i-1}-y_i) \tag{A.1}$$

With constant relative volatility, the equilibrium is computed by:

$$y_{i,j} = K_j x_{i,j},\ K_j = \frac{\alpha_j}{\sum_j \alpha_j x_{i,j}} \tag{A.2}$$

Where index j is component number.

The liquid out of the tray is a function of holdup and vapor flow. A linearized approximation is used, and holdup is computed by a differential equation:

$$\begin{aligned} L_i &= g(M_i, V) \approx k_0 + k_1 M_i + k_2 V_{i-1} \\ \frac{dM_i}{dt} &= L_{i+1} - L_i \end{aligned} \tag{A.3}$$

The whole column is modeled by connecting the tray models together in sections, and by computing the flows into the sections according to the column construction in Fig. 1. We assume no vapor flow dynamics, thus $V_i = V_{i-1}$ inside a section.

The feed enthalpy factor q is here defined by:

q>1	Subcooled liquid
q=1	Saturated liquid
0<q<1	Liquid and vapor
q=0	Saturated vapor
q<0	Superheated vapor

Practical implementation of liquid split and side-stream withdrawal may involve full withdrawal of all downcomer flow into an external accumulator, and controlled flow back into the column again. The liquid and vapor splits are assumed to be realized by splitting the flows at two specified ratios:

$$\begin{aligned} L_{1in} &= R_l L_{3out} \\ V_2 &= R_v V_6 \end{aligned} \tag{A.4}$$

A.2 Nomenclature

B	Bottom product flow	z	Feed composition
D	Top product flow	u	Control input vector
F	Feed flow	f,g,h	functions
K	K-factor	t	time
L	Liquid flow	w	Material flow
N	Number of trays	α	Relative volatility
R_l	Liquid split fraction		
R_v	Vapor split fraction	Subscripts	
S	Side-stream flow	a,b,c	Component a,b,c
T	Temperature	D,S,B	Product streams
V	Vapor flow	F	Feed stream
q	Feed enthalpy factor	i	Tray number (1=top)
x	Composition, state	j	Component (a,b,c)
y	Measurement vector	1-6	Section numbers

A.3 Column Data

6 tray sections with 8 stages each. Connected as shown in Fig. 1.
Relative volatilities $\alpha_{a,b,c}$ =4:2:1. Feed with three components, nominal values: F=1, q=1 (liquid feed), $[z_a,z_b,z_c]$=[1/3,1/3,1/3],
Nominal setpoint is 0.97 for all product purities (mole fraction of main component in product). For dynamic simulations: Nominal holdup, M_0=1.0. Holdup for sections 3 and 6 is M_0, and $M_0/2$ for section 1,2,4 and 5. Holdup for condenser accumulator is $10M_0$. Holdup for liquid split accumulator and side-stream accumulator is set to M_0. (Thus very small accumulators are assumed here.) Holdup values does not affect steady state properties. Hydraulic factor: k_1 = 4.0 (which gives a liquid time-constant of 0.25 min. for each tray, and a total delay of approximately 8 min. from top to bottom), k_2=0. Bias terms are set to match a specific steady state flow through a section. Time unit: M_0/F_0 = 1 min.