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DYNAMICS AND CONTROL OF INTEGRATED THREE-PRODUCT (PETLYUK) DISTILLATION COLUMNS

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Abstract : This paper considers operation and control the Petlyuk design. The degrees of freedom are analyzed especially at steady-state. These results together with steady-state solution curves help describe the complex plant dynamics and possible optimization strategies. We also propose control schemes for controlling three and four product compositions. The results indicate that there may be serious problems involved in operating the Petlyuk column, at least for high-purity separations.

1 INTRODUCTION

The separation of more than two components has traditionally been done by arranging distillation columns in series. Several alternative configurations exist, most notably the direct and indirect sequence (where light or heavy components are removed first, respectively).

Almost 50 years ago Wright (1949) proposed a promising design alternative for separating a ternary feed. This design consists of an ordinary column shell with the feed and sidestream product draw divided by a vertical wall through a set of trays.

It is usually denoted a Petlyuk column after Petlyuk et al. (1965) who later studied the scheme theoretically. Many authors have later predicted considerable savings in energy and capital cost with this design, but still few of these integrated columns have been built. One reason is probably that the Petlyuk column, compared to an ordinary distillation column, has many more degrees of freedom in both operation and design. This undoubtably makes the design of both the column and its control system more complex.

A two-column implementation of the Petlyuk design is shown in Figure 1. It consists of a prefractionator with reflux and boilup from the downstream 3-product column, a setup with only one reboiler and one condenser. As proposed by Wright (1949) practical implementation of such a column can be accomplished in a single shell by inserting a vertical wall through the middle section of the column, thus separating the feed and side product draw. Petlyuk's main reason for this design was to avoid thermodynamic losses from mixing different streams at the feed tray location. We will hereafter denote the product streams D, S and B (and feed F), with ternary components **1**, **2** and **3**. Molefractions are denoted x_{ij} where i is the stream and j is the component.

A similar design, but with a condenser and reboiler also for the prefractionator was proposed even earlier by Brugma (1939). We will denote this a pseudo-Petlyuk design.

As compared to the direct or indirect sequence, this implementation of the Petlyuk design offers savings in investment (only one shell and two exchangers) as well as operating costs. Although several authors have studied the design of such columns, very little work has been done on the operation and control.

Stupin and Lockhart (1971) claimed that Fenske-Underwood design computations overestimated the stage requirements and found the performance of the Petlyuk column to be rather insensitive to changes in trays and internal flows.

Tedder and Rudd (1978) were among the first to study the optimal separation of a given ternary feed. The alternatives included the direct and indirect sequence, columns with sidedraws, columns with sidestrippers and siderectifiers and a pseudo-Petlyuk design. They found the pseudo-Petlyuk design to be preferable when

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the fraction of intermediate component **2** in the feed is large (40% - 80%).

Cerda and Westerberg (1981) derived simple methods for estimating the operating parameters at limiting flow conditions.

Fidowski and Krolikowski (1986) compared the optimal (minimum) vapor flow rates for the direct and indirect sequence with both the Petlyuk and the pseudo-Petlyuk design. The Petlyuk design shows significant savings. The developed analytical expressions are based on the Underwood formulas.

Glinos and Malone (1988) also derived analytical expression for various alternative designs, including the Petlyuk design. Their recommendations are to use the Petlyuk design when the fraction of intermediate component **2** in the feed is small, and they found that the maximum vapor savings compared to simple sequences were about 50% when $x_{F2} \rightarrow 0$. They found that columns with siderectifiers may be equally well suited when less the fraction of component **2** in the feed is less than 30%. However, they concluded that Petlyuk columns may also have a significant advantage for moderate or high x_{F2} values, but that the conclusion depends on the relative volatilities.

Chavez et al. (1986) discuss the possibility for multiple steady states in complex columns, concentrating their work on a Petlyuk design. The found that the Petlyuk design has five degrees of freedom at steady-state, and they found that four different steady-state solutions may occur when specifying three purities (in each of the products) plus bottom rate and reboiler duty. They explain this in terms of matching specifications in interlinked columns.

Faravelli et al. (1989) build on the work of Chavez et al. and look at which of the steady states are most resilient to changing internal flows. They applied "control" to the column, but only to aid in finding the steady-state solutions.

Triantafyllou and Smith (1992) present a good overview over the design of Petlyuk columns, and explain how it may be approximated as a regular column with two sidestrippers which are joined together.

The only report of an industrial implementation of a Petlyuk design is from BASF in Germany (as reported by Rudd, 1992)

In this work we will study the dynamic behavior of a Petlyuk column and propose suitable controller structures.

The original motivation of this project was to study composition control of the three product streams of a Petlyuk column. The results from this study, which are presented at the end of this paper, show that from a linear point of view there are no major problems.

However, during this work it became clear that there are serious problems related to the steady-state behavior that can make practical operation very difficult. The main problem is that there exist "holes" in the operating region for which it is not possible to achieve the desired product specifications. This behavior has no equivalent in ordinary two-product distillation columns.

2 DEGREES OF FREEDOM

We here consider the *Degrees of Freedom* in a given column with fixed stages, feed locations, etc., here abbreviated to DOF.

Starting with binary distillation and considering steady-state where it is assumed that the holdups (condenser level, reboiler level and pressure) are already controlled, two independent (manipulated) variables remain, for example L and V.

In a Petlyuk column we get at steady-state three additional degrees of freedom - one for each of the three additional streams leaving the column. These are the sidestream S plus the streams L_1 and V_2 sent back to the prefractionator (we will use the fractions $R_L = L_1/L$ and $R_V = V_2/V$ as DOFs in the further analysis). Note that in this analysis the prefractionator itself does not have any degrees of freedom at steady state. The five DOFs for the Petlyuk design may be used to specify (control) the top and bottom composition (x_{D1} and x_{B3}) and one or two compositions in the side stream. This leaves one or two degrees of freedom for optimization purposes, which we in this paper select to be minimizing the energy consumption in terms of the heat duty Q_B.

There are also possibilities for increasing the DOFs, for example, by taking off several sidestreams (e.g., a vapor and liquid sidestream, S_V and S_L), and by using a triple-wall solution as suggested in the figure in the paper of Petlyuk et al., but these are not considered here.

In a usual two-product distillation column one can at most control one specification for each product (two-point control). Simpler alternatives are no control (relying on self-regulation) or one-point control. Since in high purity distillation columns it is critical that the overall prod-

uct split is adjusted correctly (such that D/F is approximately equal to the fraction of light component), one generally finds that no control is unacceptable. However, due to strong interactions one-point control, with the composition in the other end being self-regulated, is usually satisfactory if some over-refluxing (increased energy consumption) is allowed for.

For a Petlyuk scheme one must at least adjust two product splits correctly (e.g. D/F to match the light component and S/F to match the intermediate component), thus at least two-point control is required. Such a control scheme is not treated in detail here, but again it is clear that it will at least require increased energy consumption. Additionally, there will be no way to adjust the separation in the prefractionator, as determined by the recycle fractions R_L and R_V.

In this paper we first study three-point control where one composition in each product is controlled, for example x_{D1}, x_{S2} and x_{B3}. This may be an adequate control scheme.

However, with only one degree of freedom to control the sidestream composition, we will not be able to adjust the ratio between the sidestream impurities, x_{S1} and x_{S3}, which may constitute an additional product specification. Thus, we finally consider four-point control with four product composition specifications (two in the sidestream).

3 CASE STUDY

Previous authors have looked at a variety of ternary systems, from close boiling C_4 isomers to component sets spanning C_1 to C_6. We have chosen the system ethanol, propanol and butanol for the examples. This system has a relative volatility of approximately 4:2:1 for the three components.

Steady state simulations were done with ASPENPLUS, using Redlich-Kwong-UNIFAC thermodynamic properties. Optimization, linearization and dynamic simulations were performed with SPEEDUP, assuming constant molar flows and constant relative volatility. This model incorporates linearized flow dynamics with a time constant of 3.6 minutes. Although the thermodynamic data are different, the programs have yielded very similar results.

We have used the same number of trays in the center sections of the "main" column as in the prefractionator. This is in line with the assumed industrial implementation with a dividing wall in the shell. The "main" column consists of 40 stages and there are 20 stages in the prefractionator. The feed is liquid with a flowrate of 60 *kmol/min.* and feed composition $x_F = [0.33, 0.33, 0.33]$. We demand 99% pure products in the top and bottom and the design purity in the sidestream is 99%.

Design	Boilup
Direct	100 %
Indirect	108 %
Rectifier	88 %
Stripper	89 %
Pseudo-Petlyuk	85 %
Petlyuk	**77 %**

Table 1: Relative energy consumption.

Economic gain in Petlyuk design. Earlier work has showed that the Petlyuk design often is more energy efficient. This was confirmed for our mixture and the savings in energy compared to the standard "direct sequence" with two columns was 23%. As shown in Table 1 it was also favorable compared to other schemes. These were the **Indirect** sequence, removing the heaviest component first, **Pseudo-Petlyuk**, as described earlier and a binary column with a side-**Rectifier** or side-**Stripper** attached, respectively. All designs consist of 60 stages, optimally distributed between the design column section. The designs have been optimized to give the least boilup.

4 STEADY STATE

4.1 Four compositions specified

As noted above the column has five degrees of freedom at steady-state. We first study the steady-state behavior with four compositions specified: $x_{D1} = 0.99$, $x_{B3} = 0.99$, $x_{S2} = 0.99$ and $x_{S1}/x_{S3} = 1$ (99% purity for each product and equal distribution of the impurities in the sidestream). The purity of the sidestream (x_{S2}) is nominally 0.99, but the results are also given for other values.

One degree of freedom (DOF) then remains to be specified (denoted X in the following). For operation it is important to make a good choice of X since this variable will be kept constant or changed only slowly to minimize the operation costs, which is here selected to be given by the heat duty, Q_B. At first we expected to find a

relationship as given in Figure 2, where Q has a minimum as a function of X. Ideally, we would like the plot to be as "flat" as possible such that the exact value of X was not too important.

Unfortunately, the picture is not quite as simple in practice. This is illustrated in Figure 3 which shows Q_B as a function of $X = R_L$ (the internal reflux ratio to the prefractionator) for two values of x_{S2}. The first thing to note is that there for some values of R_L are two possible solutions. One of these corresponds to a higher value of Q_B and should be avoided. These results are similar to those of Chavez (1986). Thus, if R_L is used as the DOF to be kept constant, the first challenge for operation and control would be to stay at the "lower" solution corresponding to the smallest Q_B. Assuming that this could be done, we find for $x_{S2} = 0.986$ that keeping R_L at about 0.35 would be a good choice, and that Q_B would not depend too strongly on the exact value. However, for increased sidestream purity, $x_{S2} = 0.99$, there is a "hole" in the operating region, and for $R_L = 0.35$ it is not possible to achieve the desired product specifications even with infinite reflux.

It is then clear that R_L is not a good choice for the remaining DOF. To see if other choices are better we prepared similar plots for other choices ($X = R_V$, compositions in the prefractionator. See Figure 3-6). However, we find that none of these are acceptable. For example, with R_V fixed we find a hole in the operating range for *low* values of x_{S2}. We also find similar problems when specifying compositions in the prefractionator.

4.2 Three compositions specified

The conclusion from the above plots is that "holes" in the operating range will make it very difficult to control four compositions. A possibly better alternative is to control only three compositions, that is, to let the ratio of the impurities in the sidestream vary freely (and not specify $x_{S1}/x_{S3} = 1$ as above). This yields another DOF that must be specified, for example, one may select $X_1 = R_L$ and $X_2 = R_V$. This is the choice made in the control part later.

We have not make extensive studies with only three compositions fixed, but obviously the removal of one specification "loosens up" the problem somewhat, and one may at least reduce the holes in the operating range. Reducing the constraints on the system will probably move the "holes" to operating points with higher purity products.

For example, while it was impossible to achieve $x_{S2} = 0.99$ with $R_L = 0.35$ and $x_{S1}/x_{S3} = 1$, we find that we can achieve $x_{S2} = 0.99$ with $R_L = 0.35$ and $R_V = 0.50$, for example, giving $x_{S1}/x_{S3} = 1.23$ and $Q_B = 87.5MW$.

5 CONTROL

In the remaining part of the paper we consider control of the column using decentralized control. The reflux (L) is used to control top composition (x_{D1}), boilup (V or Q_B) is used to control bottom composition (x_{B3}), and sidestream flowrate (S) is used to control sidestream composition (x_{S2}). For "three-point" control R_L and R_V are fixed. For "four-point" control R_L is used to control the impurity ratio (x_{S1}/x_{S3}) with R_V fixed.

5.1 Linear Analysis Tools

In the following we will use a plant description of the form

$$y(s) = G(s)u(s) + G_d(s)d(s) \qquad (1)$$

where G and G_d denote the process and disturbance plant model and y, u and d are the measurements, manipulated inputs and disturbances, respectively.

In this paper we mainly use the relative gain array (RGA or Λ) to look at interaction in the distillation column. The properties of the RGA are well known (e.g., Grosdidier et al., 1985). The most important for our purpose are: 1) No twoway interaction is present when $\Lambda = I$, 2) The RGA is independent of scaling in inputs or outputs, and 3) The rows and columns both sum up to 1. To evaluate the disturbance sensitivity, we consider the closed loop disturbance gain (CLDG) which is the appropriate measure when we use decentralized control (Hovd and Skogestad, 1992). The CLDG is defined as $\Delta = G_{diag}G^{-1}G_d$, where G_{diag} consists of the diagonal elements of G. For decentralized control frequency-dependent plots of δ_{ik} may be used to evaluate the necessary bandwidth requirements in loop i, that is, at low frequencies the loop gain $L_i = g_{ii}c_i$ must be larger than δ_{ik} in magnitude to get acceptable performance.

We also look at the singular value decomposition $G = U\Sigma V^T$ and examine the elements of G.

The disturbances considered are changes in the feed flow and feed composition.

All variables have been scaled with respect to the maximum allowed change: $\Delta L = \Delta V = 30\%$, $\Delta R_L = \Delta R_V = 0.2$, $\Delta S = 25\%$, $\Delta x_{ij} = 0.01$, $\Delta F = 17\%$ and $\Delta z_F = 20\%$.

5.2 Linear analysis, three-point control, LVS-configuration

In this case R_L and R_V are fixed and the outputs and inputs are

$$y = \begin{pmatrix} x_{D1} \\ x_{B3} \\ x_{S2} \end{pmatrix} \quad u = \begin{pmatrix} L \\ V \\ S \end{pmatrix}$$

The Petlyuk column at the operation point with minimum energy use ($R_L = 0.394$, $R_V = 0.55$) has no poles or transmission zeros in the right half plane (RHP). Thus, there are no fundamental problems with instability, inverse responses or inherent bandwidth limitations.

RHP zeros may occur between S and x_{S2} for other operating points, depending on how the sensitivity of the sidestream compositions varies. Changes in S will affect on x_{S3} somewhat as an integrator, while changes in x_{S1} will level off after a short time. The initial slope for these two responses will determine if an inverse response occurs or not.

The steady state gain matrix G is

$$G(0) = \begin{pmatrix} 112.9 & -112.6 & 0.112 \\ -85.3 & 86.6 & 14.5 \\ 28.4 & -26.8 & -9.70 \end{pmatrix}$$

We see that the sidestream S mainly affects the middle and bottom product, while both L and V have a large effect on x_{S2}. We see quite readily that there will be interaction between the top and bottom composition, in line with ordinary binary distillation.

The singular value decomposition $G = U\Sigma V^T$ (at steady-state) will allow us some conclusions on the high and low gain directions of the plant. The output and input directions are given in U and V, respectively and the singular values are $\Sigma = diag[297 \quad 15.0 \quad 0.64]$.

$$U = \begin{pmatrix} 0.72 & -0.68 & 0.16 \\ -0.69 & -0.69 & 0.21 \\ 0.03 & 0.26 & 0.97 \end{pmatrix}$$

$$V = \begin{pmatrix} 0.65 & -0.04 & 0.76 \\ -0.76 & 0.03 & 0.65 \\ -0.05 & -1.00 & -0.02 \end{pmatrix}$$

We see that the high gain direction corresponds to moving the top and bottom compositions in opposite directions, or moving the column composition profile up or down. The low gain direction corresponds to moving them in the same direction, i.e. making both D and B more or less pure. This is in accordance with ordinary distillation. The medium gain direction corresponds almost entirely to changing S and moves x_{S2} opposite to x_{D1} and x_{B3}.

We then look at the interaction and disturbance rejection properties. The steady state RGA values

$$\Lambda(0) = \begin{pmatrix} 26.19 & -25.19 & 0.00 \\ -32.65 & 32.83 & 0.82 \\ 7.47 & -6.64 & 0.17 \end{pmatrix}$$

show again that the control of x_{D1} and x_{B3} interact. The same trend is evident from the frequency dependent RGA as shown in Figure 7. The interaction tapers off at higher frequencies, showing that the control having effect around the bandwidth of the plant will not be much affected by interaction.

The closed loop disturbance gain, CLDG, is shown in Figure 8. The most difficult disturbances to reject are changes in F on x_D and x_B requiring a bandwidth of about 0.25 rad/min (time constant of 4 minutes) in this loops. On the other hand, the required bandwidth for controlling x_{S2} is significantly smaller (less than 0.1 rad/min).

5.3 Nonlinear simulations

The conclusion is that from a linear point of view the process is easy to control in this operating point. This is confirmed by the nonlinear simulation in Figure 9 which shows the closed loop response to disturbances in F ($60 \rightarrow 50$) and z_F ($[0.33, 0.33, 0.33] \rightarrow [0.33, 0.40, 0.27]$) and a distillate purity setpoint change ($0.99 \rightarrow 0.995$), respectively. However, a setpoint change in x_{S2} of $0.99 \rightarrow 0.995$ is infeasible for this operating point, showing that three-point control may have problems for some range of R_L and R_V. The response of x_{S1} and x_{S3} to a setpoint change in x_{S2} help explain why the column has more difficulties with increased purity specifications in the sidestream than in the top or bottom. This is due to x_{S1} being insensitive to changes in S. Thus an increase in x_{S2} will primarily reduce x_{S3}, which becomes increasingly difficult at high x_{S2} values. This leads to an interest in four-point control, including x_{S1} or x_{S3} as measured variable.

5.4 Four-point control, LVR$_L$S configuration

R_L is added as a manipulated variable and is used to control x_{S1}. The set of measurements and manipulated variables is thus

$$y = \begin{pmatrix} x_{D1} \\ x_{B3} \\ x_{S1} \\ x_{S2} \end{pmatrix} \quad u = \begin{pmatrix} L \\ V \\ R_L \\ S \end{pmatrix}$$

The process gain and RGA at steady-state operating conditions are

$$G(0) = \begin{pmatrix} 124.67 & -124.48 & 0.09 & 0.11 \\ -118.86 & 119.31 & -0.09 & 20.02 \\ 23.44 & -23.64 & -0.09 & -0.21 \\ 5.82 & -5.16 & 0.01 & -4.30 \end{pmatrix}$$

$$\Lambda(0) = \begin{pmatrix} 25.69 & -24.80 & 0.11 & 0.00 \\ -32.92 & 33.04 & 0.06 & 0.82 \\ 0.71 & -0.56 & 0.85 & -0.00 \\ 7.52 & -6.68 & -0.02 & 0.17 \end{pmatrix}$$

We see that although a suitable pairing exists ($L \rightarrow x_{D1}$, $V \rightarrow x_{B3}$, $R_L \rightarrow x_{S1}$ and $S \rightarrow x_{S2}$) the manipulated variable R_L has a very low gain towards *all* control objectives. The largest gain is about 0.1 which means that the input signal needed to reject disturbances will be approximately 10 times the assigned bounds. The closed loop disturbance gain is nearly identical to the three-point control case. The additional measurement x_{S1} is insensitive to all disturbances, having values below 0.2 at all frequencies and thus not needing control at all for disturbance rejection. Conclusion: x_S1 is insensitive to both inputs and disturbances. This confirms the steady-state analysis where we found that specifying the ratio x_{S1}/x_{S3} may not yield feasible solutions.

5.5 Problems with Four-point control

It was predicted earlier that four-point control may experience problems with either R_L or R_V fixed. This is indeed the case, and Figure 10 shows the result of a setpoint *decrease* in x_{S2} with fixed $R_V = 0.525$; the column becomes unstable. The difficulties with operating in areas corresponding to "holes" in the $Q_B(X)$ plots seriously limit four-point control, despite good disturbance rejection properties.

6 CONCLUSION

The Petlyuk column displays complicated behavior with multiple internal distributions for given product compositions. Some product specification sets may be infeasible ("holes") for some choices of R_L and R_V in the operating range. It has been shown that fixing R_L or R_V at values in the "hole" may give instability to x_{S2} setpoint increases *and* decreases, respectively. A better understanding of the complexities of the Petlyuk column is needed.

The results have illustrated that it is possible to control a Petlyuk column, although serious problems may arise due to the mentioned "holes". Three-point control looks most promising.

There is an abundance of DOFs when counting both design and control and all have not been exploited here. For example, the stage for withdrawing S heavily influences x_{S1}/x_{S3}. The design of the Petlyuk column is a difficult task and developments here may aid the operational problems encountered.

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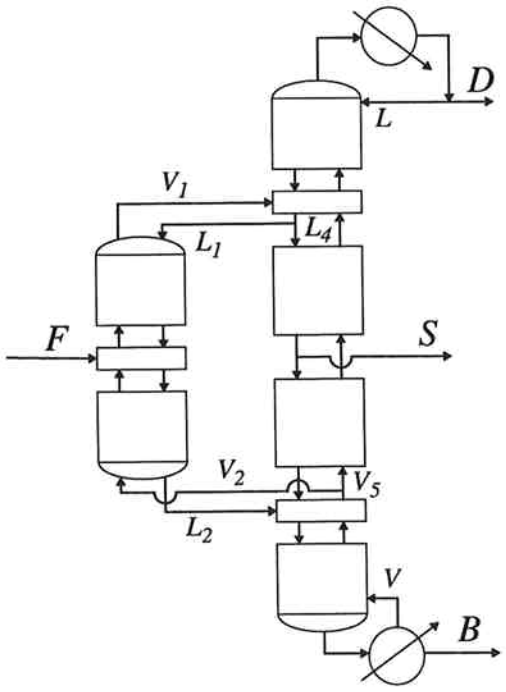

Figure 1: Petlyuk column stream notation.

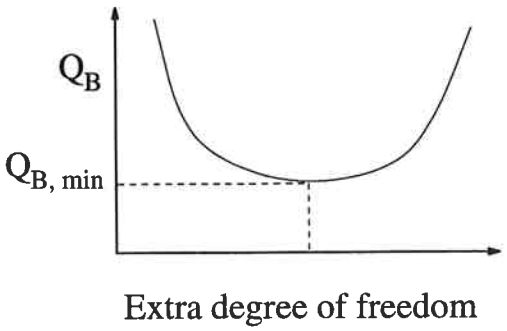

Figure 2: Energy use (Q_B) as function of extra DOF.

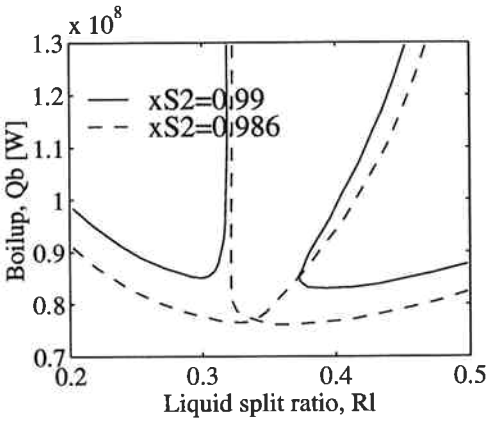

Figure 3: Energy use as a function of R_L (four compositions specified).

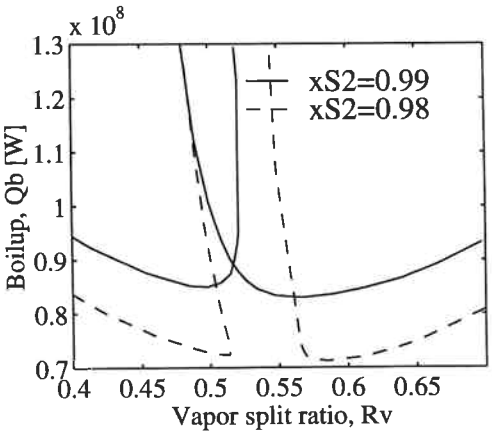

Figure 4: Energy use as a function of R_V (four compositions specified).

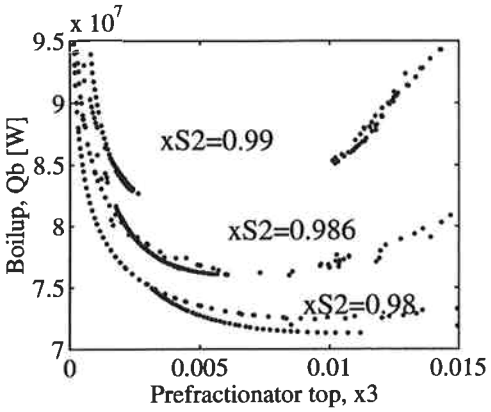

Figure 5: Energy use as function of composition of component 3 in prefractionator distillate.

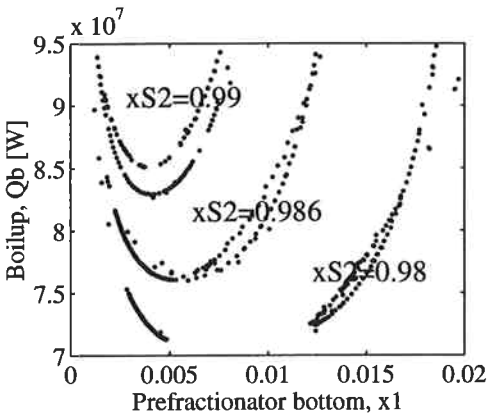

Figure 6: Energy use as function of composition of component 1 in prefractionator bottoms.

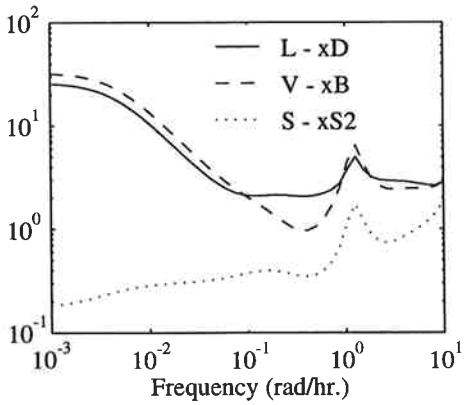

Figure 7: Relative gain array, λ_{ii} for LVS configuration.

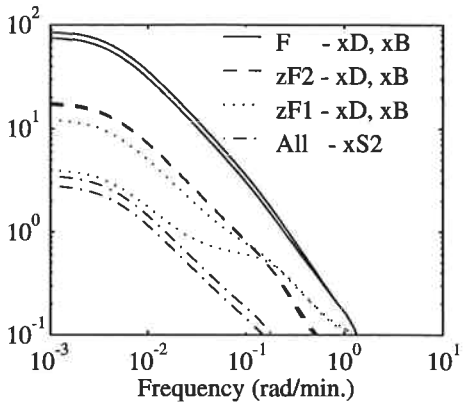

Figure 8: Closed loop disturbance gain, δ_{ij}, for LVS configuration.

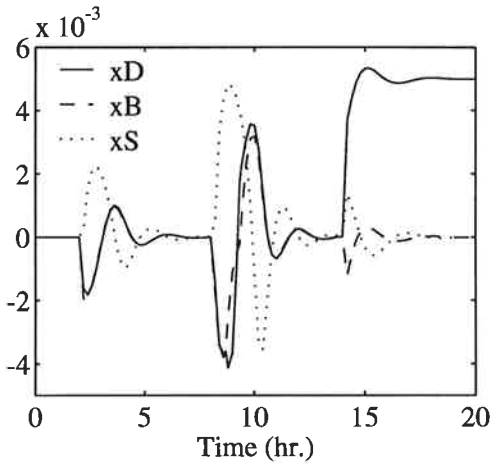

Figure 9: Time response to disturbances and setpoint change, LVS configuration.

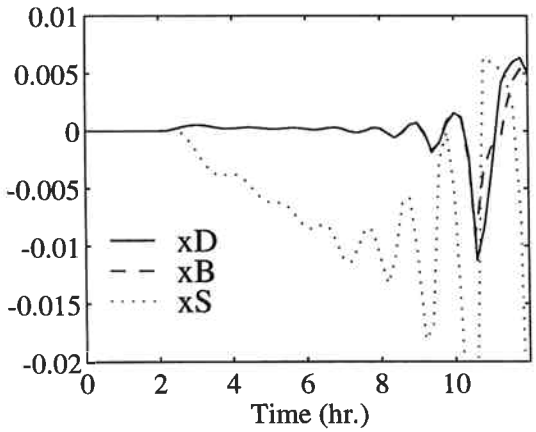

Figure 10: $x_{S2} = 0.99 \rightarrow 0.98$ setpoint ramp decrease from $t = 2$ to $t = 7$, LVR$_L$S-configuration.