Estimators for Product Composition in Distillation Columns

by

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NOMENCLATURE.

B - Bottom product flow rate
d - disturbances
C - Controller
D - distillate flow rate
EPV - Explained Prediction Variance.
F - feed flow rate
F_i - Gain matrixes from inputs to secondary measurement (temperatures)
G_i - Gain matrixes from inputs to primary outputs.
K, k_0 - estimator constants
L - reflux flow rate
L_θ - logarithmic temperatures based on reference temperatures
M_B, M_D, M_V - Holdups in the column, see Fig 1.1.
M_θ, M_y - Transferfunctions of measurement device.
PCR - Principal Component Regression.
PLS - Partial Least Square Regression.
q_F - fraction liquid inn feed
RGA - Relative gain array, (Bristol, 1966)
t - principal component (score), latent variable
T - matrix of scores
T^b - boiling temperatures of pure component
u - manipulated inputs $(= (L, V)^T)$
v - process noise (disturbance)
V - boilup rate from reboiler
V_T - overhead vapor flow
W_i - weight functions for temperature scaling
x - mole fraction of light component
x_B - mole fraction of light component in bottom product
y - output vector $= (y_D, x_B)^T$
y_D - mole fraction of light component in distillate
z_F - mole fraction of light component in feed

Greek symbols

α - relative volatility
η_M - Murphree tray efficiency
$\gamma(A)$ - condition number of matrix A
μ - Structural Singular Value
ω - frequency (min^{-1})
$\sigma_i(A)$ - The i'th largest singular value of matrix A
Σ - covariance matrix
θ - temperature
Θ - data matrix of θ

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Chapter 1

Introduction

Distillation is perhaps the most important unit operation in process industry. In many plants it involves about 30–40% of the total investment and energy costs. Thus, small improvements in plant operation may imply important cost reductions. The very large number of published articles dealing with various aspects of distillation operation reflect the importance the industry and the academic community have given this subject over the years.

During the last decade greater emphasis has been placed on saving energy. This is a result of higher energy prices, but also of an increasing conscience in the community for the environmental consequences of high energy consumption. In the future it will become imperative to operate the distillation columns more efficiently with respect to energy. To do so, not only the design and operation conditions must be optimal, but also the control system involved in maintaining these optimal conditions.

Separation mixtures in distillation columns require input of energy. The energy needed for a specific column increases exponentially with the degree of separation. Poor composition control implies large periods of operation with purer products than necessary, and thereby losses of energy. Tight composition control is consequently important for energy savings. It will also give larger profits in terms of product recovery.

1.1 Distillation Control.

Figure 1.1 displays a binary distillation column with one feed and two product streams. The control objectives are to maintain the product compositions x_B and y_D, the holdup of reboiler and accumulator, M_B and M_D, and the pressure, P, at desired levels. The manipulable variables available are the distillate D, the bottom product B, the reflux L,

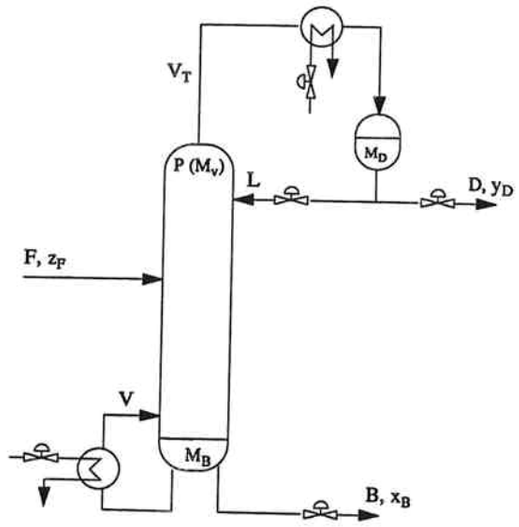

Figure 1.1: Distillation column with 5 manipulated inputs (L,V,D,B and V_T) and 5 controlled outputs (y_D, x_B, M_D, M_B and P).

the boilup V, and the overhead vapor flow V_T. The latter two are manipulated through reboiler and condenser duties.

The five inputs and the five outputs to the plant give rise to a multivariate (5×5) control problem. One might think that this problem is best solved by a full multivariable (5×5) controller taking all possible interactions among the variables into account. But, since the liquid and vapor dynamics turn out to be much faster than the composition dynamics, the holdups (M_B, M_D and P) are easily controlled by three single loops. Actually, the most common control practice is to use single PID-loops for the product compositions as well. This is quite surprising, since distillation columns are known to have large interactions among these compositions loops. However, this gives less complex and more robust control systems, which are also easier to understand and tune for the operators. This practice is also found, at least for some examples, to be quite close to optimal (Skogestad and Lundstrom, 1990). The reason is that the distillation columns with large interactions are ill-conditioned (high condition numbers and large RGA-values), that is, the process gain is strongly dependent on the input direction (combination of inputs).

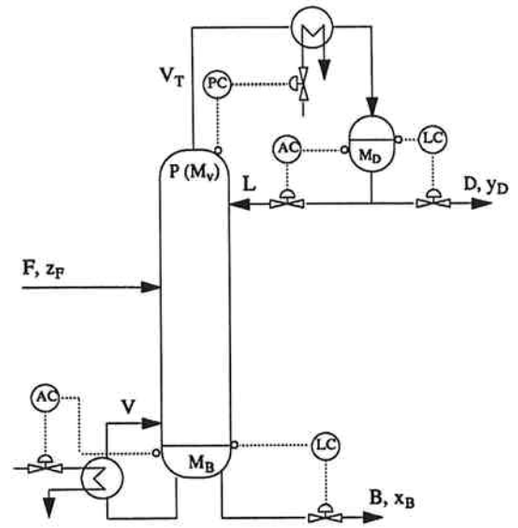

Figure 1.2: Distillation column with LV–configuration.

Inverse based controllers, e.g. decouplers, will then be very sensitive to uncertainties in input and model.

Using five SISO-controllers, the next question is how to pair the input variables with the output variables. The pressure is usually controlled by the condenser duty. The four remaining variables may be paired in a lot of different ways. The different configurations are denoted after which of the two manipulated inputs that are used for composition control. The two most common configurations are the LV-configuration, i.e. the pairing of y_D with L and x_B with V, and the DV-configuration, i.e. the pairing of y_D with D and x_B with B. The liquid holdups are controlled by the remaining inputs.

The selection of configuration is an important control issue which is extensively discussed in the literature, e.g. Shinskey (1984), Waller (1986), Skogestad and Morari (1987), Waller et al. (1988) Skogestad et al. (1990). In this thesis, however, where the focus is on the estimation problem, the selection is far less important, although not always irrelevant. In this thesis the LV-configuration has been chosen mainly because it seems to be the most common configuration, but also because it in some sense is the most "basic" configuration. L and V have a direct influence on the compositions in the column, while

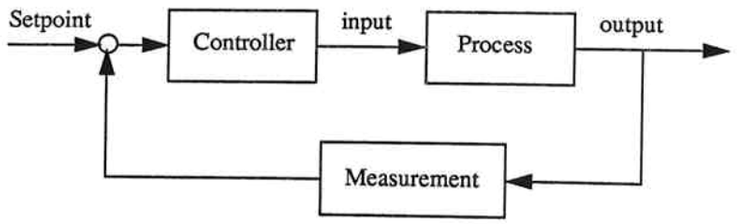

Figure 1.3: General control loop.

D and B have more indirect influence through the control loops of the reboiler and accumulator levels. The LV-configuration yields also a very ill-conditioned plant which is of interest from a theoretical point of view.

Many industrial columns are today operated with one-point control of the product compositions, i.e. only one of the composition control loops is closed. The reason may be constraints on one of the inputs, or simply that the one-point control is a much easier control problem to handle because one then omits the interaction problem connected with two-point control. In this thesis, however, it is implicitly assumed that two-point control is to be used.

Figure 1.2 shows a typical implementation of the LV-configuration.

1.2 Product composition measurement.

The control loop consists of the process, the measurement device, and the controller. (Fig. 1.3). Each part should be designed with the other two in mind. A constraint or a fault in one part will affect the performance of the whole system. For instance, a substantial bias in the measurement device will normally have a damaging effect on the control effort, no matter how sophisticated the controller is. In the following, the measurement problems for distillation columns will be addressed.

The measurement of pressure and liquid levels is performed by pressure or differential pressure sensors. These sensors are quite robust and easy to maintain. The placement and implementation of the sensors may, however, sometimes involve problems, but this

subject will not be considered here. (It is well covered for instance in Buckley et al., 1985, p 256–273).

The measurement of the compositions is generally much more difficult. Among on-line analyzers the gas chromatographs are most common, but also infrared and ultraviolet analyzers, mass spectrometers, boiling point analyzers, flash point analyzers and refractive index analyzers are in use (Rademaker et al., 1975). Ideally, the analyzer method chosen should be sensitive only to the actual component such that other components and physical conditions do not interfere. This objective is often difficult to meet under practical circumstances. The result is that frequent calibrations become necessary. If the interfering conditions are changing periodically they will be especially troublesome to handle. The sampling and sample conditioning are also week spots. Troubles such as two-face sampling and plugging or partial phase changes in the sampling lines happens quite frequently (Kister, 1990). All these matters often imply high maintenance costs. One employee for every third analyzer may be typical for gas chromatographs.

For safety reasons the analyzers are often placed in separate control rooms some distance away from the column. This gives additional measurement delays. With gas chromatographs, a typical overall measurement delay then becomes 10 to 20 minutes, which may imply serious control limitations.

These drawbacks of on-line composition measurement are the main reasons why most distillation columns are still using temperature for composition control. Temperature control is cheap, easy to maintain, fast in response to composition changes, and may be measured continuously. Of course, the use of temperature also implies difficulties. These will be discussed in the following chapters.

1.3 Brief survey of the thesis.

The thesis addresses the use of multiple temperatures for composition estimates. Chapter 2 and 3 will give a literature survey of this subject. Chapter 2 deals with basic principles of temperature control, that is, how to keep some temperatures, or simple functions of them, constant at some trays in the column. Chapter 3 will deal with the use of temperature in model based product composition estimators.

Chapters 4, 5 and 7 contain the main results of the thesis. They are written as articles and may thus be read separately. In Chapter 4 three different types of estimators (Kalman, Brosilow, Regression) are compared in a linear study. Chapter 5 discusses

several refinements of the most promising of them, the regression estimator. This study involves nonlinear simulations and evaluation of the estimated predictive ability. Chapter 7 gives the results of an implementation of the regression estimator on a pilot plant distillation column.

Chapter 6 contains a description of the experimental column and the associated equipment. Finally, Chapter 8 gives a summary of the results and discusses some possible directions for future work.

All references cited in this thesis are listed after Chapter 8, at page 148. At the end of each article (Chapter 4, 5 and 7) there are separate lists of references and symbols as well. For the other chapters please refer to the list of symbols at the beginning of the thesis.

Chapter 2

Temperature control.

This chapter is divided in two parts. The first part addresses the basic principles of using single temperature measurements, including the important issue of sensor location. The last part contains various means of dealing with the weak spots of temperature control by using additional temperatures.

2.1 Use of single temperatures.

The use of temperature to infer composition is based on the assumption of thermodynamical equilibrium between liquid and vapor on the trays in a distillation column. At a given pressure, P, there exists a unique boiling point temperature, θ_b, corresponding to a specific liquid composition, x

$$\theta_b = f(x, P) \tag{2.1}$$

Assuming constant pressure and equilibrium conditions, a temperature measurement will consequently infer a binary composition exactly. In multicomponent systems, however, the temperature is not a true composition indicator since different mixtures may have the same boiling point temperature.

2.1.1 Pressure compensated temperatures.

Changes in pressure caused by changes in setpoint, inaccuracies in the column pressure control, or changes in pressure drops in the column from varying column loads will influence the temperature measurements according to equation 2.1. One common way to compensate for the influence of pressure, is to obtain a measurement of the pressure. A pressure compensated value of the temperature, θ, is then used as input to the controller,

e.g.

$$\theta_{PC} = \theta - \left.\frac{\delta\theta}{\delta P}\right|_x \Delta P \tag{2.2}$$

This linear compensation is sufficient in most cases.

2.1.2 Problems with temperature measurements.

Consider for the moment a binary mixture with compensated temperatures. Accurate temperature measurements at the top and the bottom tray in the column will then be exact for composition estimation. However, different kinds of disturbances may affect the temperature measurement:

- Noise and offsets associated with the measurement and data treatment device. This includes the inaccuracy of the pressure measurement and the compensation.
- Temperature variations due to flow pulses and improper mixing on the trays.
- Temperature offsets due to improper equilibrium conditions.

2.1.3 Sensitivity.

The sensitivity-to-noise ratio of the measurement device is often a critical factor. If the temperature span caused by the changes in the compositions is small compared with pressure fluctuations and measurement noise, the use of temperature for composition control will become very difficult. One problem with distillation columns is that the temperature variations are very small at the end of the column near the bottom product and the distillate. This is due to the often extremely pure product compositions. However, the temperature changes are much larger towards the middle of the column. Consequently, the temperature sensors are usually moved to a location where the sensitivity is large enough. According to Thurston (1981), the temperature change should be about $0.1 - 0.5\,^{\circ}\mathrm{C}$ per % change of the manipulated variable for the control tray (steady state changes).

2.1.4 Correlation with the products.

The reason why a tray some distance away may be employed for control is that the temperatures on trays located close to each other are very correlated through the mass and energy balances. However, the further the temperature measurement is from the ends, the weaker is the correlation with the product composition, because the effect of

the compositions of the other end and the feed will then increase. Keeping a temperature constant will no longer keep the product composition constant.

2.1.5 Non-key components.

When the system is multicomponent the influence of the non-key components will make temperature control much more difficult. However, there are usually sections in the column where the non-key compositions are rather constant. On the other hand, at the end of the column, the temperature will be dominated of the separation between the non-key and the pure key component. These places should, therefore, be avoided for temperature control (Rademaker et al., 1975).

2.1.6 Measurement location.

The issue of temperature location has been extensively discussed in the literature. The most important criteria have been the *sensitivity* and *correlation* criteria discussed above, and for multicomponent distillation also the influence of non-key components. Other criteria employed are considerations of dynamic and linearity properties of the control loop, and minimum interaction between the loops. However, these matters are usually less important because they may be often handled by the control system.

Among the textbook authors in distillation control theory, Buckley et al. (1985) are the only ones who argue strongly for placing the measurements at the ends. The only exception they find is when it is practically impossible (which according to the authors is seldom with present-day measurement technology). On the other hand, Nisenfeld and Seeman (1981), Shinskey (1984), and Desphande (1985) pay much more attention to the sensitivity criteria. They argue that there frequently appear situations where placing the temperature away from the ends is both necessary and favourable, for instance in high purity columns and in multicomponent systems. This will be the case irrespective of the measurement technology.

2.1.7 Procedures for measurement location.

Since measurement selection/location is a general problem encountered in many processes, a lot of general procedures have been proposed to deal with this problem, (e.g. Morari and Stephanopoulos, 1980; Jørgensen et al., 1984; Ghosh and Knapp, 1989; Lee and Morari, 1989.).

For the temperature location in distillation columns, several additional procedures have been proposed, e.g. Tolliver and McCune (1980), Yu and Luyben (1987), and Moore et al. (1987). These procedures focus mainly on the sensitivity criteria. The latter two involve Singular Value Decomposition (SVD) on the steady state process matrices between inputs and temperatures. Yu and Luyben (1987) use the gain matrix from the disturbances to temperatures, while Moore et al. (1987) use the gain from inputs D and V to the temperatures.[1] The main idea is to use corresponding column vectors in the right and the left singular matrices. The largest element in each vector are paired, i.e. the dominating input with the dominating output (temperature) for each singular value. This method seems intuitively reasonable, but may yield very arbitrary results if the right singular matrix has large non-diagonal elements (for instance for the LV-configuration).

A main drawback with many procedures is that they do not include noise and disturbance characteristics of the column. The solutions often are based on either the sensitivity criteria or the correlation criteria, which of course gives these procedures a limited validity. In Chapter 5 a method for measurement selection is proposed that has much in common with the SVD-method, but which does not suffer from the same weaknesses.

2.2 Use of several measurements.

In order to improve the temperature control, several methods which involve additional measurements have been suggested. One frequently used extension is the differential temperature control.

2.2.1 Differential temperatures.

The effect of overall pressure changes (not pressure drops) may be compensated for by the use of differential temperatures. Since the column pressure has about the same effect on all temperatures in the column, an additional temperature measurement (preferably located at a tray where the composition is almost constant) will primarily track the pressure variation. The temperature difference will then be a selective measure of the composition changes.

One drawback is that the relationship between differential temperature and the product composition usually has a point of inflection (Niesenfelt & Seeman, 1981). However,

[1] They used the condition-number as an additional criterium to prevent some solutions that gave too strong interaction between the loops.

if the range of composition changes is not very large, this is usually not a problem.

A lot of authors (e.g. Waller and Finnerman, 1987) discuss the use of sums and differences between two temperatures in the column instead of single temperatures. This is, however, not a method to improve the measurements, but rather an attempt to counteract interaction between the loops.

2.2.2 Double differential temperature control.

Luyben (1969) proposed to use an additional differential temperature in the same section to take care of the pressure drop changes in the column as well. Boyd (1975) reports a successful industrial implementation of this scheme.

Use of two differential temperatures was also proposed by Yu and Luyben (1984) to infer feed composition changes in a multicomponent system. One was selectively sensitive to the key components, the other to the most important non-key components. The temperatures were used to reset the setpoints of two ordinary temperature controllers. In a simulation study they found that this control scheme was better than the Brosilow inferential control (Joseph and Brosilow, 1978a). Only feed composition changes were considered; the feed flow rate disturbances were supposed to be handled by some ratio system, e.g. steam to feed. How this feed-forward control system affected the temperature control was not discussed.

2.2.3 Temperature profile control.

This application was first proposed by Luyben (1972) for columns with sharp temperature profiles. They are characterized by high relative volatility and high product purity. Most of the mass transfer will then take place in a rather narrow section in the column. The centre of the profile will move up and down the column when the product composition is changing. A sum of temperature measurements located on different trays will be able to track this centre, and the product composition is supposed to be controlled by keeping the centre at a desired position (tray).

A similar approach has been implemented on three towers (a deethanizer, a demethanizer, and a C_2-splitter) by Johnson (1984), and on a C_2-splitter by Whitehead and Parnis (1987). They used a weighted temperature average of differential temperatures as input to the controller.

Bozenhardt (1988) used temperature profile control on an azeotrope distillation of

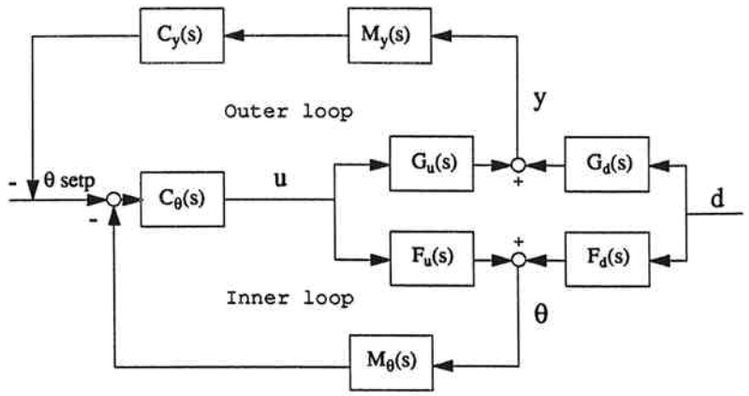

Figure 2.1: Parallel Cascade Scheme.

alcohol/water/ether column. Instead of a sum or an average, the maximum temperature differences between two trays was measured and used as input to the position controller.

2.3 Hybrid control scheme: Parallel Cascade.

Figure 2.1 shows a quite frequently employed cascade scheme, involving both a gas chromatograph and a temperature sensor. It is denoted as parallel cascade control (Luyben, 1973), because the manipulative variable (e.g. L) affects the composition and the temperatures through two transfer matrices in parallel. (This is a property of the process, and the control structure is a cascade.) It uses the temperature, which is sampled frequently, as an inner control loop, while the infrequent composition measurement is used to update the setpoint of the temperature loop. It thus takes advantage of both the fast temperature control and the more accurate analyzer control. To yield good performance, the temperature loop must be tuned fast enough to take care of the main disturbances before the outer loop starts adjusting the setpoint. Otherwise the loops may counteract each other and give instability problems (Kister, 1990).

Alternatively, Bartman (1981) proposed a scheme to deal with this interaction problem by involving a composition predictor which predicted the effect of the temperature control

action on the composition. This effect was subtracted from the composition analyzer measure before entering the outer loop controller.

The cascade system is a good alternative when both accurate and fast control is necessary. Compared to the analyzer control it also has the advantage of giving control action during analyzer breakdowns. The main disadvantages with this system are the interaction problem for slow temperature loops, and most importantly, the costs associated with composition analyzers.

Chapter 3

Model based estimators.

Since the control objective is to keep the product compositions, rather than some tray temperatures constant, a more appropriate means of using temperatures is for composition estimation, and let the estimates be the input to the controller.

To build an estimator, some kind of a process model is needed. The level of sophistication of the estimator will depend on the model complexity involved. The choice of estimator will, therefore, often be a trade-off between performance and development costs.

The following presentation of estimators for distillation columns will be restricted to those reported for distillation columns in the literature.

3.1 Static estimators.

Linear static estimators are the simplest and easiest to handle since their models consist of only constant matrices.

3.1.1 Inferential Estimator.

In the early seventies Brosilow and co-workers proposed to use secondary measurements in an estimator that inferred the product compositions. In 1978 the concept of "Inferential Control" was introduced in connection with this estimator. The basic idea is to use the secondary measurements, such as temperature and input flows, to infer all unknown disturbances, and then to perform a kind of feed-forward disturbance rejection control. Although the method is general, Brosilow and co-workers have mainly discussed its application to distillation columns.

Weber and Brosilow (1972) claimed that a static estimator could yield a satisfactory

dynamic performance for a class of processes. A method to decide when the process was within such a class was not given, but they claimed that typical situations were when the disturbances varied gradually and moved the process from "one steady state to another through a sequence of steady states". One example was a distillation column with very slow disturbances in feed rate and feed composition.

Consider the following linear steady-state model of the column in terms of deviation variables:

$$y = G_d d + G_u u \tag{3.1}$$

$$\theta = F_d d + F_u u \tag{3.2}$$

Here the dependent variables are the outputs y (compositions) and secondary measurements θ (temperatures). The independent variables are the disturbances d, e.g. (F, z_F) , and manipulated inputs u, e.g. (L,V).

From eq. 3.2 an estimate of the disturbances is obtained

$$\hat{d} = F_d^{\dagger}(\theta - F_u u) \tag{3.3}$$

where $F_d^{\dagger}$ denotes the pseudo-inverse of F_d.

The estimate of y is

$$\hat{y} = G_u u + G_d \hat{d} \tag{3.4}$$

If *the number of measurements is equal to or larger than the number of disturbances*, the least square expression of the pseudo-inverse is:

$$F_d^{\dagger} = (F_d^T F_d)^{-1} F_d^T \tag{3.5}$$

One restriction to this estimate is that $(F_d^T F_d)$ must be nonsingular, i.e. the rank must be equal to the number of disturbances. A linear relationship between the disturbances will violate this restriction. In that case, Weber and Brosilow (1972) recommended to reduce the number of *disturbances in the model.*

In Joseph and Brosilow (1978) the estimator expression for the case of *more disturbances than temperatures* is given. In this case we have

$$F_d^{\dagger} = G_d(F_d F_d^T)^{-1} \tag{3.6}$$

In the paper the derivation is based on stochastic theory and is as follows: Let the disturbances be jointly distributed random vectors. Let y_d and θ_d be the part of y and θ

that is due to the disturbances, i.e.

$$y_d = y - G_u u = G_d d \tag{3.7}$$

$$\theta_d = \theta - F_u u = F_d d \tag{3.8}$$

Since y_d and θ_d also are random vectors the best linear least square estimator of y_d from θ_d is (Rhodes, 1971):

$$\hat{y}_d = \Sigma_{y_d\theta_d}\Sigma_{\theta_d\theta_d}^{-1}\theta_d \tag{3.9}$$

$$\hat{y}_d = G_d\Sigma_{dd}F_d^T(F_d\Sigma_{dd}F_d^T)^{-1}\theta_d \tag{3.10}$$

where Σ denotes the covariance matrix. Redefining the disturbances such that Σ_{dd} is the identity matrix gives Eq.(3.6).

An implicit assumption for the Eq.(3.10) is that the matrix $(F_d\Sigma_{dd}F_d^T)^{-1}$ is nonsingular. This will not be the case if there exists strong couplings between the temperature measurements. Problems are also expected if the matrix is close to singularity. Weber and Brosilow (1972) showed that the estimation error is directly related to the condition number of F_d. A high condition number[1] means that the expression above is close to singular, and the estimator will be very sensitive to small model errors. Joseph and Brosilow (1978) recommended to *reduce the number of temperatures* such that the condition number is less than 100. They suggested a temperature selection procedure based on 1) small condition number and 2) small estimation error.

Two drawbacks of the inferential estimator for distillation columns in the present form are quite apparent:

1. The matrices G_d, G_u, F_u and F_d must be modelled carefully since the method seems to be quite sensitive to modelling errors.

2. Temperatures (or possibly disturbances) have to be deleted in order to reduce this sensitivity.

In the Inferential Control scheme the estimator is used in a kind of feed-forward scheme, see Figure 3.1.

Lee and Morari (1989) proposed another selection procedure for the inferential control based on the μ-analysis of Doyle (1982). Compared to the one of Joseph and Brosilow

[1]See chapter 5, section 3.1

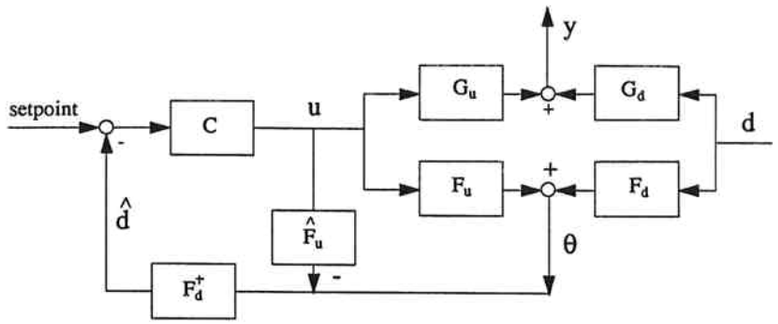

Figure 3.1: Inferential control system.

(1978), this procedure is more rigorous. However, also this procedure minimizes a kind of condition number, and only a few of the available temperature measurements are selected. In Chapter 4 we show that additional measurements generally improve the estimates and make them less sensitive for different measurement locations.

Patke et al. (1982) did a comparison of the inferential and the parallel cascade schemes by a simulation study of a multicomponent system. They found that the inferential control had some steady state deviations, but was much faster in response to disturbances. However, the comparison has some obvious weaknesses: For the cascade scheme the liquid sampling is after the accumulator tank, and tuning of the analyzer PI-loop is "trial and error". An integral time of 0.07 h for the inner loop and 0.10 h for the outer loop, indicates that this cascade scheme also suffers from interaction problems.

In Patke and Deshpande (1982) an evaluation of the inferential control was performed on an experimental binary column and compared with a one-temperature control. The steady state deviation of the two systems was about the same, but the settling time of inferential control was about half that of the temperature control.

3.1.2 Multivariate Regression Estimators.

In multivariate regression analysis (See, e.g., Mardia et al., 1979) the estimator is obtained by a training set of known values of y and θ.

Let K denote the linear estimator between p y-variables and q θ-variables

$$y = K\theta \tag{3.11}$$

The vectors y and θ in eq. 3.11 are assumed to be centred (deviation variables).

The n different runs in the training set are lined up in two data matrices, $Y^{n\times p}$ and $\Theta^{n\times q}$, such that the measurements of each run are placed in one row. We then have:

$$Y = \Theta K^T \tag{3.12}$$

The ordinary least square solution for K is:

$$K_{OLS} = Y^T\Theta[\Theta^T\Theta]^{-1} \tag{3.13}$$

This corresponds to eq. 3.9, i.e.

$$K = \Sigma_{y\theta}\Sigma_{\theta\theta}^{-1} \tag{3.14}$$

since $\Sigma_{y_d\theta_d} = \frac{1}{n}(Y^T\Theta)$ is the covariance matrix for y and θ and $\Sigma_{y_d\theta_d} = \frac{1}{n}(\Theta^T\Theta)$ is the covariance matrix for θ in the calibration runs. The matrix $\Theta^T\Theta$ must be nonsingular, i.e. the matrix Θ must have the full rank of q. This requires that $n > q$ and that the q measurements are linearly independent. This restriction corresponds to that of the Brosilow estimator, and implies that only a limited number of measurements may be included.

In Joseph et al. (1976) the inferential estimator was compared with the regression estimator. Only steady state calculations were performed and no noise was included. They concluded that the inferential estimator using five measurements was better than those using four or six, and that the regression estimator was slightly worse in all cases.

The comparison has, however, some obvious weaknesses. Specifically, logarithmic transform of the compositions was used in the case of inferential control, but not for the regression estimator. This logarithmic transform linearizes the plant gain matrices and improves the estimate. There were also different temperature locations for the two estimators.

A comparison with a nonlinear regression estimator, i.e. a linear regression with quadratic and product terms of the temperatures, was performed as well. The nonlinear estimator was found to have very poor performance. The reason is, although not stated in the paper, that this estimator has 17 coefficients (compared to 6 for inferential estimators), and implies a very ill-conditioned regression problem using ordinary least square.

Choo and Saxena (1987), after considering different kinds of model based estimators, including the inferential estimator, ended up with an implementation of a regression estimator on an extractive distillation column. The main reason was the small development costs connected with this estimator. Based on historical data, this estimator used four temperatures and a pressure measurement. Later on, an additional measurement of the feed composition was included. Large improvements in control performance were reported.

Improved regression methods.

There are, however, better ways of handling the collinearity problem encountered in the regression estimator than by using a limited number of measurements. Two such methods that handle the collinearity problem in a systematic way are the Principal Component Regression (PCR) and Partial Least Square (PLS) (See Martens and Næss, 1989). The principal idea of these methods is to find a small number of "latent variables", i.e. linear combinations of the temperatures which reflect the influence of main physical quantities affecting the temperatures, and use those in the regression step. These latent variables are selected such that they are mutually orthogonal. The methods are described in Chapter 5, section 3, and are extensively used in the thesis.

The PCR method employs the singular value decomposition (SVD) of Θ and deletes the small singular values corresponding to noise. Similarly, SVD should be employed on the process gain matrix F_d in the Brosilow scheme to yield a better conditioned estimator. This will avoid deleting temperature measurements or disturbances.

3.1.3 Nonlinear estimators.

Distillation columns are known to be nonlinear, and linear estimators will only be valid close to the linearization point. To build estimators which are valid for a larger range of operation is therefore important.

Luyben and co-workers developed a rigorous nonlinear estimator, first for binary systems (Shah and Luyben, 1979), and later for multicomponent systems (Yu and Luyben, 1987). In a n-component system they used feed rate, feed temperature, distillate product rate, and $n-1$ temperatures as input to a rigorous tray by tray calculation procedure, which estimated all compositions and temperatures on the trays. In a closed loop simulation study this static estimator was compared to a composition analyzer for step changes in feed composition. For typical computer times and analyzer delays they found that the estimator performed best. The estimator was, however, found to be somewhat sensitive

to uncertainty in the measurements.

This method employs only the absolute minimum number of temperatures. In a binary system this will involve only one temperature! However, including additional temperatures may strongly reduce the effect of the noise and model-plant mismatch. In particular, the estimate may be very sensitive to the value of $\frac{D}{F}$ (fraction distillate to feed rate).

Rhiel and Krahl (1988) used a much simpler nonlinear model on an industrial column. On a selected tray some distance away from the end, the binary composition was first found from a temperature and a pressure measurement. This composition was then in turn used together with measurements of the reflux and boilup to estimate the product composition. They assumed a linear equilibrium line and constant molar flows, but they included a variable tray efficiency, using a experimentally found correlation between the efficiency and the loads.

3.1.4 Alternative handling of nonlinearity.

Much of the nonlinearity in distillation columns may be alternatively handled by logarithmic transforms, for instance as proposed by Joseph et al. (1976), for the product compositions. Also the concentration profiles will be linearized by using logarithmic transforms, e.g. the logarithmic transform of the separation parameter

$$X = ln\frac{x_L}{x_H} \tag{3.15}$$

will yield a nearly straight line against tray number, unless there are pinch zones around the feed tray. Linear models using logarithmic transformed variables may, therefore, apply for quite a wide range of operation conditions.

3.1.5 Problems with using flow measurements in static estimators.

A critical question concerning the static estimator is how they perform dynamically. The time responses of the compositions on the different trays are very similar, in particular for flow changes, (Skogestad and Morari, 1988a), and consequently the temperatures will have much the same dynamics as the product compositions. On the other hand, the dynamics between the compositions and the flows or the pressures are quite different, and the claim of Weber and Brosilow (1972) that a static estimator may yield satisfactory performance, will not apply for estimators including these measurements. Using static

estimators with flow measurements is, therefore, not recommended, without doing some kind of dynamic compensation or filtration. Both Brosilow and Luyben introduce lead-lag elements to improve their estimators (Brosilow and Tong, 1978; Yu and Luyben, 1987). However, this requires additional modelling effort, and may introduce additional sources of model-plant mismatch.

3.2 Dynamic estimators.

3.2.1 Kalman filter.

The most popular dynamic estimator is undoubtedly the Kalman filter. It was developed in the early sixties (Kalman, 1960; Kalman and Bucy, 1961) and is an integral part of the traditional optimal control theory. This estimator contains a full dynamic model of the plant, and the estimated states are corrected using gain feedback from the measurements. The estimator is optimal in the sense that it minimizes the expected variance of the estimated states. The Kalman filter is described in Chapter 4 section 2.1, and a comprehensive survey of theory and applications is found in Sorenson (1985).

There seems to be very few implementations of Kalman filters for composition estimation in distillation columns. However, some simulations and experimental studies have been done in connection to optimal (LQ) control, see e.g. Waller (1982). The Kalman filter has also become a kind of "standard" estimator for comparison with other estimators in simulation studies, e.g. Tong and Brosilow (1978).

The main drawback with the Kalman filter is probably that it is time consuming to implement and initialize, and that it yields a heavy computer load. Another drawback is that it requires a very good model in order to prevent divergence problems (Griffin et al., 1988).

3.2.2 Dynamic estimators for distillation columns

The more recent literature dealing with dynamic estimators for distillation columns consists basically of two research groups, one in Stuttgart, Germany, and one in Newcastle upon Tyne, Great Britain.

The Stuttgart group.

The group consists of Gilles and co-workers. Gilles and Retzbach (1980), picked up the idea of tracking the temperature profile control proposed by Luyben (1972). An

azeotrope distillation of isopropanol and water using an extractant was considered. The column had a sidestream which mainly consisted of the intermediate component water. Besides controlling the product compositions, it was desirable to keep the concentration of water at its highest value at the tray where this sidestream was located. Two temperature fronts were identified, one caused by the high mass transfer region of isopropanol/water and the other of extractant/water. Their position in the column, together with heat input, vapor stream and feed disturbances were used as state variables in a linear state space model. This model gave rise to two different estimators; an observer and a Kalman filter. The optimal feedback controller was combined with feed-forward control of feed rate and feed composition, the latter estimated by the observer.

The tracking of the temperature profile is used quite nicely to optimalize the sidestream product. However, the profile tracking takes care of only the main dimension in the column, the split. Profile changes caused by changes in compositions in the feed or at the other end will not be tracked. In this particular column, however, the feed was taken care of by feed-forward control, and the other end had little influence because of pinch zones around the feed trays.

In Marquardt (1986), Marquard and Gilles (1988), and Marquard (1988) these ideas are developed further to generalize all types of distillation columns. Although the composition profile is not particularly sharp, it does move up and down the column by stream changes. The location of the front, the maximum slope of the profile, is a state variable together with some shape parameters and product compositions. According to Marquard, the shapes generally do not change much, they are mainly a function of the equilibrium line. The equilibrium line may be parameterized, and the shape constants calculated. The model is used in a stationary Kalman filter (Marquard, 1988), and tested in a nonlinear binary simulation study with feedback.

This approach is more rigorous than that of Gilles and Retzbach (1980), since it also tries to track the other dimensions in the concentration profiles by introducing additional shape parameters.[2] However, as already stated, most of the concentration profile shape disappears when using logarithmic scales, so the concept of temperature front is somewhat over-emphasized.

Lang and Gilles (1989) use a nonlinear observer model which calculates temperatures, pressures, liquid and vapor compositions on each tray. The model is based on mass

[2]But since it is stressed that these parameters do not change much, they do not seem well suited for the purpose.

transfer fluxes equations, and assumes that the mass transfer resistant is on the vapor phase side.

The temperature measurement is placed at the same spot as the desired location of the temperature front. The deviation between the calculated and measured temperature is used as feedback to correct the mass transfer flux on all trays in the model. The feedback gain, however, is proportional to the mass transfer flux on each tray. In binary systems the proportional constant is the only parameter to tune. Otherwise, an additional parameter and temperature measurement are required for each component extra.

The Newcastle group.

Guilandoust et al. (1986) use a linear dynamic SISO-estimator to estimate the product composition. The other input is considered as disturbance, so one-point control is probably assumed. The estimator is supposed to cope with the slow time varying plant parameters by use of primary measurements. The parameters are not modelled, but updated recursively each time a primary measurement is available, i.e., a kind of adaptive estimator where only the structure is modelled.

In the paper they compare two different approaches, one starting with a state space description, the other directly derived from an input-output model. In the state space description they start with the innovation form of the model and transform it to an observer canonical form. In the input-output model the noise is modelled as a stationary process driven by zero mean white noise sequences. Both models end up with a similar structure, although the latter has some additional parameters due to the more rigorous noise model.

The models are tested in a simulation study for steps in feed rate and boilup. The conclusion is that the estimators perform equally well, but the input-output estimator has some more transient errors due to the additional parameters. However, the best control performance is obtained by using a combination of estimator and adaptive controller.

In Morris et al. (1988) the estimator is tested on an industrial distillation column, but the results are not very good. The temperatures are sampled every five minutes and the composition measurements every 20 minutes, but still the estimates are lagging about 20 minutes after the composition measurements! The simulation example in the paper is the same as the one used in Guilandoust et al. (1986) and Guilandoust et al. (1987).

The simulation studies suffer from not considering feed composition disturbance. The often encountered difficulties with blow-ups of adaptive schemes is not discussed either.

3.3 The use of input variable in estimators.

A common characteristic of most all estimators in the present literature about composition estimators, is that they make extensive use of flow data. If the plant is ill-conditioned, which distillation columns often are, this implies that the sensitivity for input uncertainty and model-plant mismatch are great (Skogestad and Morari, 1987). A main drawback of the literature so far, is that the consequences for the estimator performance of using uncertain input flow data, is not treated. This matter is, therefore, given greater attention in the following chapter.

Chapter 4

Output estimation for ill-conditioned plants using multiple secondary measurements: High-purity distillation

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Abstract

Temperatures and flows are often used as secondary measurements to estimate the product compositions (outputs) in distillation columns. The problem is characterized by strong collinearity (correlation) between the temperature measurements, and often between the effects of the inputs on the outputs. In a linear study three different estimator methods, the Kalman-Bucy Filter, Brosilow's inferential estimator, and Principal Component Regression (PCR) are tested for performance with mu-analysis. It is found that use of input flow measurement has a damaging effect on the estimator performance for this ill-conditioned plant (with high RGA-elements). This is the main reason why the Brosilow inferential estimator is found to perform poorly. Somewhat surprisingly, it is found that the static PCR-estimator performs well compared with the dynamic Kalman filter. The reason is that the temperatures and compostions have very similar dynamic responses. Contrary to some claims in the literature, it is found that the performance of the estimate, even when used for feedback control, generally is improved by adding temperature measurements. For high purity distillation columns and other plants with large elements in the (appropriately scaled) gain matrix, the use of input measuremets are not recommended in the present of input disturbances.

4.1 Introduction

This paper addresses the estimation of process outputs based on multiple secondary measurements. The application chosen here is the use of temperature and flow measurements to estimate the product compositions in a distillation column. This is an interesting application which features: i) a large number of strongly coupled measurements, and ii) a large number of disturbances and inputs with similar effects on the outputs.

The use of temperature measurements for feedback control of distillation columns is quite extensively discussed in the chemical engineering literature (eg., Nisenfeld and Seeman, 1981, p. 85-95). Temperatures are usually not used because they are of interest themselves, but as inexpensive and reliable indicators of composition. One problem is that temperature is a true indicator of the tray composition only if the mixture is binary and at constant pressure. Furthermore, even at steady state the correlation between the composition on a tray inside the column and the product composition at the end is not unique; it changes depending on the feed composition and the other product composition. These problems may be partly overcome by using several temperature measurements.

Measurement selection. Many columns have temperature sensors located at about every fifth tray in the column, that is, a typical column may have 5-10 temperature measurements. In industry all these measurements are rarely used. Rather, each composition measurement is replaced by a single temperature measurement and used for single-loop feedback control. The main problem is then to find a suitable location for this temperature. According to Nisenfeld and Seeman (1981) the most important issues are, i) that the temperature should be sensitive to changes in the composition, and ii) that the correlation between temperature and composition should be insensitive to disturbances in feed composition and in flows. Since the products are often very pure the first criteria favours placing the temperature sensor away from the products. The second criteria favours placing the sensors close to the product. However, in this paper, measurement location is not an important issue. The reason is that we use several (typical five or more) temperature measurements and then estimate the product compositions. In this case the exact location is far less important than in cases where single temperature measurements are used.

Problem definition. The objective is to obtain the best estimate $\hat{y}$ of the outputs (product compositions) using all available information, $\tilde{\theta}$. In terms of deviation variables

the linear estimator may be written

$$\hat{y}(s) = K(s)\tilde{\theta}(s) \tag{4.1}$$

This estimate should be obtained based on a description of the process (nominal model and expected uncertainty), the expected noise and disturbances, and a more precise definition of what we mean by "best". In the general case $\tilde{\theta}$ should include all measured dependent variables (primary measurements, y, and secondary measurements, θ), and all known independent variables (manipulated inputs, u, and measured disturbances, d). In this paper we usually have $\tilde{\theta} = \theta$, that is, the estimate is based on only secondary measurements (temperatures). The reason is that we assume no primary measurements, no measured disturbances, and we shall show for our case that the additional information contained in u is of limited value.

In this paper we consider three different approaches to the estimation problem: i) The Kalman-Bucy Filter, ii) Brosilow's Inferential Control Method, and iii) Principal Component Regression (PCR). In the last two cases we shall base the analysis on the steady-state, and use a constant gain matrix K.

Use of separate estimator. An estimator-based control scheme for the distillation column is shown in Fig.4.1. Note that we are implicitly assuming that the controller should be separated into two parts: one estimator which condenses all the measurements into a few estimated outputs, and a "small" (in terms of number of inputs) controller which uses these estimates for feedback control (Fig. 4.2). The motivation for doing this is reliability, design simplicity and robustness. In general, this solution is suboptimal compared to using one big controller which directly uses all available measurements. The reason is of course that some information is lost when the original measurements are condensed into the fewer estimated variables. In some cases it may be shown that no information is lost and this is then referred to a separation principle. In particular, this may be the case if all the states of the system are estimated since they contain all information about the system at any given point in time. However, in this paper we shall not use all states for feedback control and therefore the separation principle does not apply. And as we in our case are estimating the actual controlled outputs, we may postulate that the performance loss caused by the separation is not a major problem.

Use all available measurements ? The statement in the problem definition above that the best estimate should be based on *all* available measurements is not as obvious as one should think. Actually, a large number of authors (eg. Joseph and Brosilow, 1978, Morari

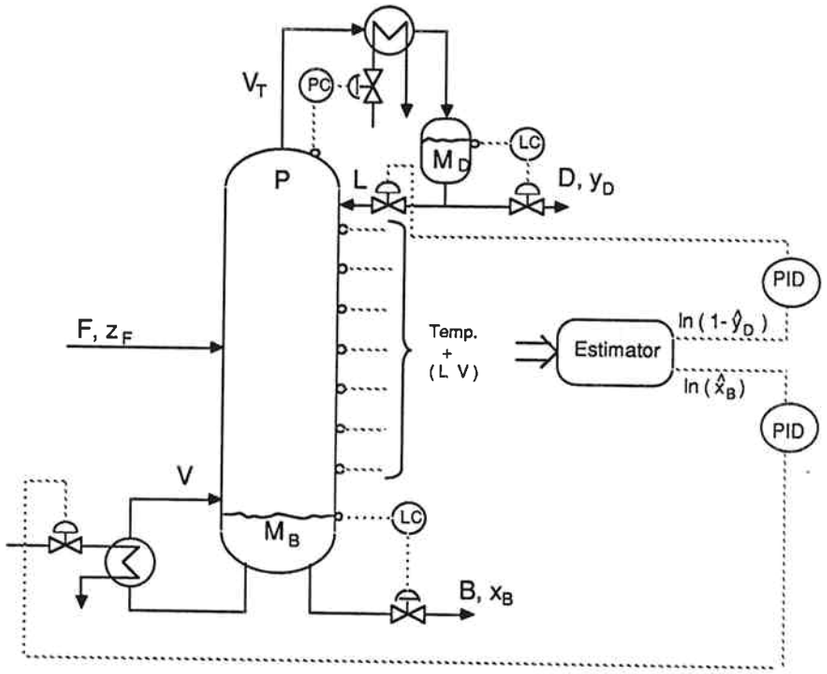

Figure 4.1: Control scheme based on LV configuration.

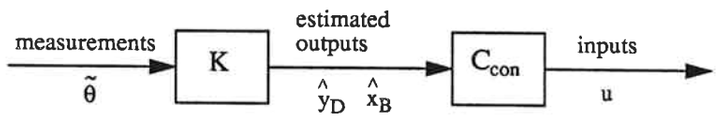

Figure 4.2: Controller block $C = C_{reg}C_{est}$ split in separate blocks for estimation and control.

and Stephanoplous, 1980, Patke et al., 1982, Yu and Luyben, 1986, Moore et al., 1987, Keller and Bonvin 1987) have suggested that one should only use a few of the *temperature* measurements to avoid the poorly conditioned problem of obtaining information from the strongly correlated temperatures. For example, our example column has 41 temperature measurements. That is, we need to determine 41 parameters in K for each output if all temperatures are used. However, the temperatures are of course strongly coupled and the 41 parameters must also be strongly coupled. Furthermore, our distillation column with two components, two products and constant pressure has only three degrees of freedom at steady state (eg., z_F, y_D, x_B). This implies that, at least for the linear case with small perturbations from the nominal operating point, we may determine at most three of these 41 parameters independently (irrespective of how the temperatures are coupled).

Latent variables. The above discussion points out the need for a robust way of obtaining the matrix K which avoids this overparameterization. Intuitively, this may be done by smoothening the available data, and obtaining a smaller number, k, of "latent variables", t, which are less coupled and contain most of the original information. These are subsequently used for estimation. In the linear case the latent variables may be written $t = P_t\theta$, where P_t is the projection matrix. The estimator then becomes $\hat{y} = K_t t$ where K_t is a "small" matrix with k parameters for each output (typically $k = 3$ in our examples), and the overparametrization in the regression step is avoided. The simplest "method", but certainly not the optimal one, is to delete measurements θ, and use, for example, only three temperatures as latent variables. This approach is implicit in some of the papers mentioned above. In Brosilows method estimated (inferred) disturbances are used as latent variables. In the PCR and PLS methods a few linear combinations of the secondary measurements are used as latent variables. These linear combinations are those which are found to be most sensitive based on the calibration set. In the Kalman estimator the states may be regarded as latent variables, although they are not independent as they are coupled through the model. Also, their number is often not less than the measurements.

Kalman estimator. The Kalman-Bucy filter (Kalman and Bucy, 1961) arises from the traditional "optimal" approach of modelling disturbances and noise as stochastic processes and minimizing a quadratic error function. This estimator contains a full dynamic model of the plant, and the states are updated using constant gain feedback from the measurements. Somewhat surprisingly, there are very few reports on the use of model-based Kalman filters for composition estimation in distillation columns. Apart from its

complexity the main disadvantage with the Kalman estimator is that model uncertainty is not included, and that it is difficult *a priori* to find the weights for the disturbance and noise.

Brosilow estimator. In process control, Weber and Brosilow (1972) proposed to use secondary measurements to estimate disturbances. Their justification is that measurement noise is usually less important in process control applications, and that the output variations are mainly caused by disturbances, which tend to vary slowly compared to the process dynamics. In Brosilows inferential controller, the disturbances are then assumed to be constant in the future, and the disturbance estimates are used in a sort of feed-forward scheme to counteract their expected effect on the outputs. We shall only use the estimator part of Brosilows scheme (Joseph et al., 1976) and not the feedback part. Brosilows scheme has a strong intuitive appeal and seems to have found some use in industry. However, because of measurement noise, model error and poor numerical properties caused by collinearity, we will show that the use of inferred disturbances as latent variables may not work well for ill-conditioned plants.

PCR estimator. A more direct approach is to derive a direct relationship between θ and y using a static regression estimator. The approach taken here is inspired by recent efforts by analytical chemists in their "multivariate calibration problem", e.g. Wold et al. (1987). This 'soft modelling' approach has an intuitive appeal to engineers as one seems to skip the modelling step: One does not have to obtain an explicit ('hard') model of how the independent variables affect θ and y (although typical variations should be included in the calibration set). Rather, one seeks a direct correlation between the available measurements (θ) and the variables to be estimated (y). However, fundamental knowledge may not be easily included in the estimator.

Analysis of estimators. The estimators are compared on a rigorous basis, considering both the estimation error $y-\hat{y}$ ("open loop" when the estimates are not used for feedback) and the control error $y - y_s$ ("closed-loop" when the estimates are used for feedback). Input uncertainty, disturbances and noise are explicitly included in the analysis using the structured singular value, μ, of Doyle (1982).

Ill-conditioned plants. The distillation column used in this paper is an example of an ill-conditioned plant. Here the plant gain is strongly dependent on the input direction, or equivalently the plant has a large condition number, $\gamma(G)$. At each frequency

$$\gamma(G) = \sigma_1(G)/\sigma_r(G) \tag{4.2}$$

α	N	N_F	z_F	y_D	x_B	D/F	L/F
1.5	40	21	0.50	0.99	0.01	0.500	2.706

- Feed is liquid.
- Constant molar flows.
- Ideal VLE using Raoults law.
- Constant pressure 1 atm.
- Holdup on each tray; $M_i/F = 0.5$ min

Parameters A,B and C in Antoine equation:
ln p(mm HG) = A - B/(T(K) + C)

Light component	Heavy component
15.8366, 2697.55, –48.78	15.4311, 2697.55, –48.78

Table 4.1: Data for distillation column example.

Here σ_1 is the largest singular value, and σ_r is the r'th (the smallest) singular value, where r is the rank of G. $\sigma_1(G)$ is a measure of the magnitude of the elements in the matrix. The smallest additive perturbation matrix which may make G loose rank has magnitude $\sigma_r(G)$. Thus, the condition number, $\gamma(G)$ gives the relative magnitude of the additive error allowed to avoid singularity (loosing rank). Consequently, matrices with a large condition number are very sensitive to numerical round-off errors (eg., Weber and Brosilow, 1972). For square matrices the relative gain array (RGA) may be used as an alternative measure. It is defined at each frequency as RGA $= G \times (G^{-1})^T$, where $\times$ denotes element-by-element multiplication. The magnitude of the RGA–elements is closely related to the optimal condition number ($\gamma(G)$ minimized with respect to input and output scaling) (Skogestad and Morari, 1987). Skogestad and Morari (1987) have shown that the RGA is also a very good indicator of how sensitive a plant's feedback control performance is to input gain uncertainty.

Example column. As an example column we use column A studied by Skogestad and Morari, 1988. The column separates a binary mixture with relative volatility 1.5, and has 40 theoretical stages, including the reboiler, plus a total condenser. Column data are given in Table 4.1. The liquid holdups are assumed constant, that is, the flow dynamics are neglected. This gives rise to a 41th order linear model in terms of the mole fraction of the light component on each tray. The two dominant time constants of the column are

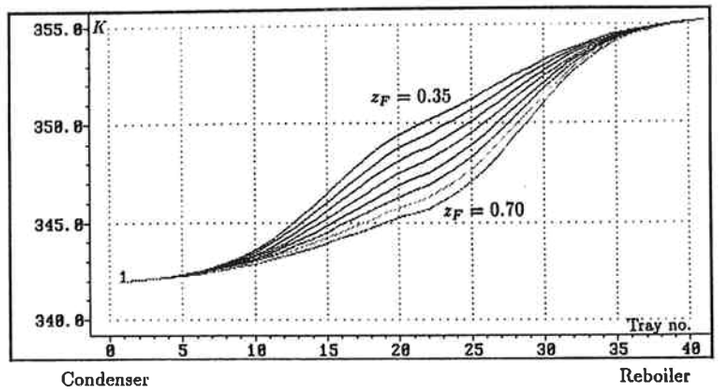

Figure 4.3: Temperature profiles for different feed compositions when y_D and x_B are held constant.

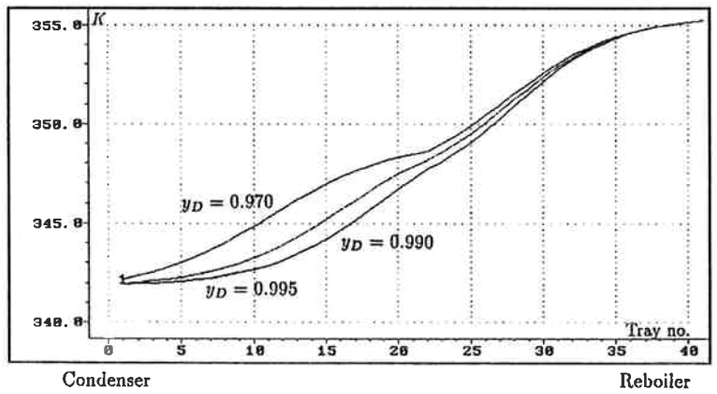

Figure 4.4: Temperature profiles for different top product compositions when z_F and x_B are held constant.

194 min and 15 min. The difference in boiling points of the two pure components is 13 °C. In Figure 4.3 and in Figure 4.4 typical temperature profiles for the column are displayed. We note that variations in temperature are small towards the ends of the columns, and that changes in feed composition have a large effect on the temperatures inside the column even though the product compositions are constant.

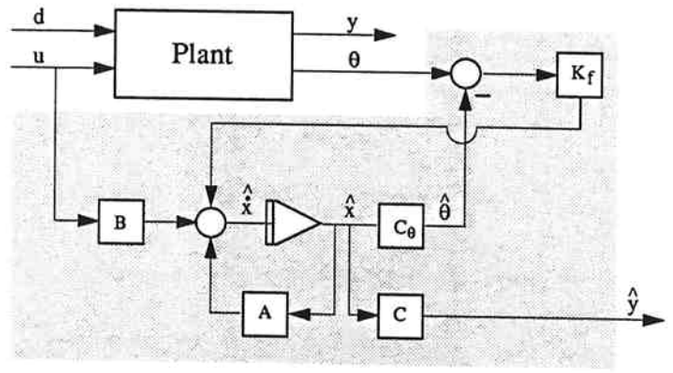

Figure 4.5: Block diagram of the Kalman Estimator.

4.2 Estimation Methods

4.2.1 Kalman filter.

In this scheme a dynamic state space model is used in parallel with the process, and the deviation between the outputs from the process and the model is used as feedback to the model through a filter gain K_f (Fig. 4.5). The linear state space model for the process is

$$\dot{x} = Ax + Bu + Ev \tag{4.3}$$
$$y = Cx \tag{4.4}$$
$$\theta = C_\theta x + w \tag{4.5}$$

Here x is the state vector, u the manipulated inputs, y the primary outputs to be estimated, θ the secondary measurements, v the process noise (disturbances), and w the measurement noise. v and w are assumed to be white noise processes with covariance matrices $\mathcal{V}$ and $\mathcal{W}$.

Minimizing the expected variance of $\theta - \hat{\theta}$ yields the estimated states

$$\dot{\hat{x}} = A\hat{x} + Bu + K_f(\theta - C_\theta\hat{x}) \tag{4.6}$$
$$= (A - K_f C_\theta)\hat{x} + Bu + K_f\theta \tag{4.7}$$

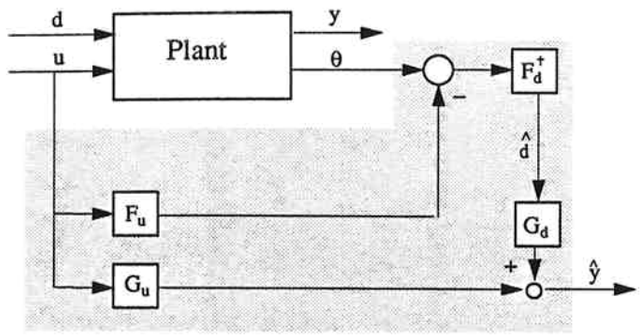

Figure 4.6: Block diagram of Brosilow Estimator.

where filter gain K_f is

$$K_f = \mathcal{X} C_\theta^T \mathcal{W}^{-1} \tag{4.8}$$

Here $\mathcal{X}$, the covariance matrix of $\hat{x}$, is found from the matrix Riccati equation

$$\dot{\mathcal{X}} = A\mathcal{X} + \mathcal{X}A^T - \mathcal{X}C_\theta^T \mathcal{W}^{-1} C_\theta \mathcal{X} + E\mathcal{V}E^T \tag{4.9}$$

We use constant filter gains which give $\dot{\mathcal{X}} = 0$, and Eq. (4.9) is reduced to an algebraic equation. The overall Kalman estimator then becomes

$$\hat{y}(s) = C(sI - A + K_f C_\theta)^{-1}(K_f \theta(s) + Bu(s)) \tag{4.10}$$

4.2.2 Brosilow estimator.

The following linear steady-state model of the column in terms of deviation variables is used

$$y = G_d d + G_u u \tag{4.11}$$

$$\theta = F_d d + F_u u \tag{4.12}$$

Here d denotes the disturbances. The matrices above are of course related to those used in the state space description in the Kalman filter. For example, $G_u = -CA^{-1}B$ and for the case $v = d$ we have $F_d = -C_\theta A^{-1} E$. Using (4.12) the estimated disturbances become

$$\hat{d} = F_d^\dagger(\theta - F_u u) \tag{4.13}$$

where the pseudoinverse $F_d^\dagger$ is the optimal inverse in the general least square sense. For the special case of more θ's than d's and independent d's (Weber and Brosilow, 1972)

$$F_d^\dagger = (F_d^T F_d)^{-1} F_d^T \tag{4.14}$$

For the special case of more d's than θ's and independent θ's (Joseph et al., 1976, Joseph and Brosilow, 1978)

$$F_d^\dagger = F_d^T (F_d F_d^T)^{-1} \tag{4.15}$$

In the general case the pseudoinverse is obtained from a SVD of F_d by deleting directions with singular values equal to zero (eg., see Strang, 1980, p. 142). Combining (4.11) and (4.13) yields the Brosliow estimator (see Fig. 4.6)

$$\hat{y} = K_B \theta + (G_u - K_B F_u) u \tag{4.16}$$

where

$$K_B = G_d F_d^\dagger \tag{4.17}$$

This static Brosilow estimator may be made equivalent to the Kalman filter at steady-state only if non-stationary noise is allowed for the disturbances v (Morari and Stephanopoulos, 1980).

4.2.3 PCR estimator.

We want to estimate p outputs (y) from q known variables (θ). The problem is then to obtain the matrix K in

$$\hat{y} = K\theta \tag{4.18}$$

To this end obtain n "calibration" sets of corresponding values of y and θ, and place these as *rows* in the matrices $Y^{n\times p}$ and $\Theta^{n\times q}$, respectively. [1] If the estimator was perfect we would have

$$Y = \Theta K^T \tag{4.19}$$

The ordinary least square solution for K is:

$$K_{LS} = Y^T \Theta [\Theta^T \Theta]^{-1} \tag{4.20}$$

which is the "regression estimator" used by Joseph et al. (1976). The $q \times q$ matrix $\Theta^T\Theta$ is n times the covariance matrix of the calibration measurements θ. This matrix is singular

[1] It might seem more reasonable to place y and θ as columns in the matrices, but we shall here use the standard notation in statistics.

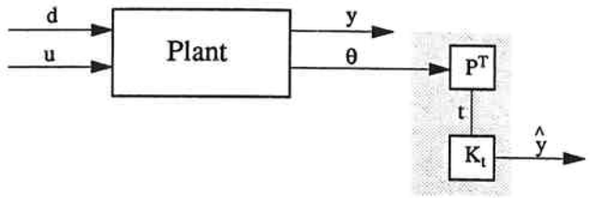

Figure 4.7: Block diagram of a PCR Estimator that does not use input information.

if $n < q$, that is, if we have too few calibration sets. It is also singular if strong collinearity in the temperatures exists. This will usually be the case in a column with measurements located close to each other.

To avoid these difficulties the general pseudo inverse in terms of the SVD is used, and directions corresponding to small singular values (principal components) are deleted. Using standard notation from the statistics literature, the SVD of Θ is written

$$\Theta = t_1 p_1^T + t_2 p_2^T + \cdots + t_m p_m^T \tag{4.21}$$

where $m \leq min(n, q)$ is the rank of Θ. Here p_1 is the eigenvector corresponding to the largest eigenvalue of $\Theta^T\Theta$, (the square of the largest singular value of Θ), and p_2 is the eigenvector corresponding to the second largest eigenvalue, and so on. The loading vectors (p's) give the directions of the principal components, while the scores (t's) give the magnitude. If all m terms in (4.21) are retained we obtain the generalized pseudoinverse. However, in PCR we select only those first k principal components that can be distinguished from the measurement noise. Let the matrices $P^{q\times k}$ and $T^{n\times k}$ include only these k most important directions. Define the new latent variables as $t = P^T\theta$. Note that $P^T = P^{-1}$ since P is orthonormal. The least square solution to $y = K_t t$ becomes $K_t = Y^T T[T^T T]^{-1}$, and the overall estimator gain matrix becomes (see Fig 4.7)

$$K_{PCR} = Y^T T[T^T T]^{-1} P^T \tag{4.22}$$

Gain		$\mathcal{V}$				
		L	V	F	z_F	
K1	diag{	200	200	0.01	0.01	}
K2	diag{	0.10	0.10	0.01	0.01	}
K3	diag{	0.01	0.01	0.01	0.01	}
K4	diag{	0.0	0.0	0.01	0.01	}

Table 4.2: Process disturbance covariance matrix of Kalman filter gains. In all cases $\mathcal{W} = 1.1\Delta\mathcal{I}$

In the general case θ may be replaced by $\tilde{\theta}$ which includes also the inputs and measured disturbances.

4.3 Estimators for the example column.

In this section we describe how the different estimators were obtained for the example column with 41 stages.

4.3.1 Kalman filter gains.

The covariance matrix of the measurement noise $\mathcal{W}$ was set to $0.04I$, where I is the identity matrix. This corresponds to $0.2\ ^\circ C$ noise on each temperature. The process noise is here defined as $v^T = [L, V, F, z_F]$ (reflux, boilup, feedrate and feed composition). Its covariance matrix, $\mathcal{V}$, was assumed diagonal and was varied in order to tune the filter. Four different values of the variance on L and V were selected (Table 4.2) and the corresponding filter gain matrices are denoted K1 to K4. The assumption of white noise process disturbances is somewhat unrealistic in a distillation column, but the estimator is not expected to be very sensitive to this assumption.

4.3.2 Brosilow estimator.

With $d^T = [z_F, F]$ and $u^T = [L, V]$, the matrices F_d,F_u,G_d and G_u in equations (4.11) and (4.12) were found by linearizing the model at the nominal operating point. The estimator was obtained using Eq. (4.16).

A modified estimator $K_{B_{mod}}$ was formed by *not* using information about the manipulated inputs u, and instead using L, V and z_f as the disturbances d' to be inferred. The

z_f	y_d	x_b	z_f	y_d	x_b
0.4000	0.9810	0.0190	0.4000	0.9810	0.0010
0.4000	0.9990	0.0190	0.4000	0.9990	0.0010
0.6000	0.9810	0.0190	0.6000	0.9810	0.0010
0.6000	0.9990	0.0190	0.6000	0.9990	0.0010
0.4500	0.9855	0.0145	0.4500	0.9855	0.0055
0.4500	0.9945	0.0145	0.4500	0.9945	0.0055
0.5500	0.9855	0.0145	0.5500	0.9855	0.0055
0.5500	0.9945	0.0145	0.5500	0.9945	0.0055

Table 4.3: Data to simulate stationary temperature profile. $q_F = 1.0$, P = 1.0 atm.

estimator then becomes $\hat{y} = K_{Bmod}\theta$ where

$$K_{Bmod} = G'(F'^T F')^{-1} F'^T \tag{4.23}$$

and F' and G' are the process matrices formed by these three variables. In the linear case with no errors in the matrices G' and F', this estimator is identical to the PCR-estimator. This is also clear if we compare (4.22) and (4.23) and imagine using changes in L, V and z_F to generate the calibration sets. In both cases we obtain the least square estimate, and if we disregard numerical problems it does not matter which latent variables we use.

4.3.3 PCR estimator.

In this paper the calibration sets are obtained from a *linear* steady state column model. A factorial design method was used to select 16 different runs around the operating point (Table 4.3). When stated random noise of magnitude 0.1 °C was added on all temperatures in the calibration sets, but the default is no noise. The specified variables were chosen as the outputs y_D and x_B and the feed composition z_F. Note that the column conditions are independent of the load (increasing all flows proportionally), and it is not necessary to simulate different feed rates. The temperature data were reduced to the desired number of principal components and K_{PCR} was computed from (4.22).

Strictly speaking, with a linear model we need only three runs (in addition to the nominal steady state) to generate the data, but we used 16 runs to better study the effect of measurement noise and to get better statistical information.

It is important to note that with this approach we may freely vary the *outputs*, y_D and x_B, and are thus able to span all directions in the output space. This is different from the Brosilow approach, which is based on an open-loop model in terms of the *inputs* (L, V, F, z_F), and where the output space will not be properly spanned for ill-conditioned plants with strongly coupled outputs y.

Case.	Location (tray no.)
41	at every tray
5a	1,12,21,30,41
5b	10,15,22,29,33
3a	2,22,41
3b	6,22,36
3c	10,22,33
3d	10,17,33
2a	1,41
2b	6,36
2c	9,33
2d	10,30

Table 4.4: Location of temperature measurements.

4.3.4 Number of measurements and their locations

The estimation methods above were applied to different locations and numbers of temperature measurements. The various cases are summarized in Table 4.4. Here tray no. 41 denotes the reboiler, no. 21 the feedtray, and no. 1 the condenser.

4.4 Analysis of the Estimators.

The objective is to evaluate the different estimation methods described above. In this section we define our criteria for the evaluation.

4.4.1 Evaluation criteria

- *Open-loop evaluation (OL).* One obvious criteria for evaluating the different estimators is their ability to follow the true composition value. The error e_1 in fig. 4.8 is the difference between the real (y) and the estimated output ($\hat{y}$). The column is assumed to operate under feedback, since this is more close to a real situation than a pure open loop test. The term "open loop" is still used since the controller uses the actual y, that is, there is no feedback from the estimate $\hat{y}$. We use single-loop PID controllers since this is the most common choice in practice. The tunings in

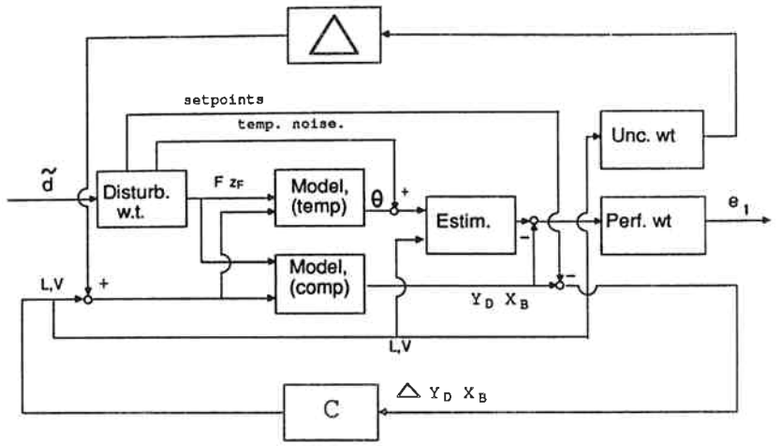

Figure 4.8: Block diagram for "open-loop" μ-test. We use $\Delta = 0$ (nominal performance) unless otherwise stated.

PID-Parameters			
Loop	K_c	τ_i	τ_d
y_D	0.589	9.53	0.620
x_B	0.555	4.42	0.332

Table 4.5: PID-parameters for the distillation column example.

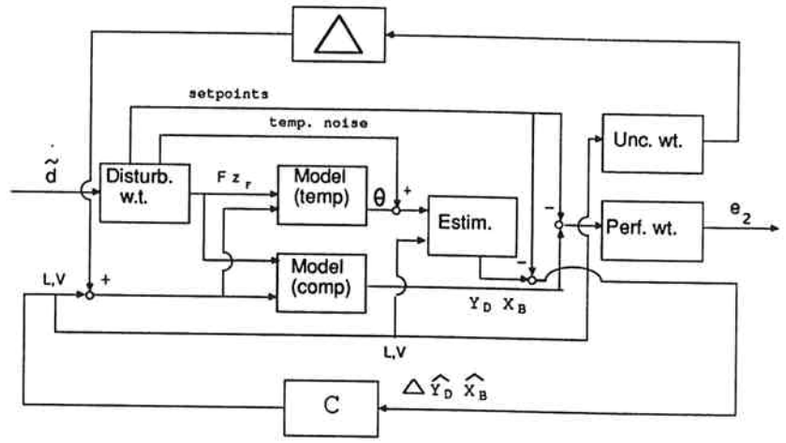

Figure 4.9: Block diagram for "closed-loop" test.

Table 4.5 yield optimal robust performance (minimize μ) when the estimate is exact. To make our results only weakly dependent on the controller used, we shall usually consider the *nominal performance* in this test, i.e., without any uncertainty. This makes the comparison independent of the robust stability requirement of the system which depends strongly on the controller.

- *Closed-loop evaluation (CL).* The main objective of the estimator is to replace the primary measurement of y, that is, use the estimate $\hat{y}$ for feedback control. The error, e_2, of interest to be minimized, is then the control error, i.e. the difference between y and y_{setp} (Fig. 4.9). We use the same controller as for the open-loop comparison, that is, a PID controller tuned optimally for perfect estimates. Using the same PID controller for all estimators will bias the comparison somewhat, as the optimal controller in each case will depend on the estimator used.

4.4.2 μ-analysis.

Our tool is the Structural Singular Value (μ) analysis (Doyle,1982). In this framework we rearrange our system to fit the general form shown in fig. 4.10. Here M denotes the generalized nominal plant including the plant and the weights, $\tilde{d}$ denotes external input

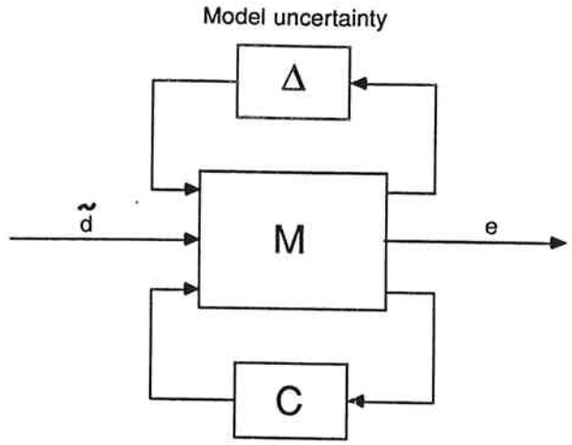

Figure 4.10: General structure for studying any linear control problem.

disturbances and setpoint changes, and e is the "error" we want to keep small. We have one Δ-block loop, which represent the model uncertainty, and one controller loop. In the μ analysis we evaluate the maximum amplification from $\tilde{d}$ to e at each frequency. Weights are used to scale the signals, $\tilde{d}$ and e, and the uncertainty Δ to be less than 1. These weights are discussed below. μ expresses the worst-case error at a given frequency, and the performance requirement for the error is satisfied if μ is less than one at all frequencies.

Uncertainty weights.

The most important source of uncertainty is assumed to be on the inputs (L and V). We shall use the same uncertainty weight as Skogestad and Morari (1988), which is given by

$$w_I(s) = 0.2\,\frac{5s+1}{0.5s+1} \tag{4.24}$$

The weight is shown graphically in fig 4.11a. In the low frequency range it allows for a 20% uncertainty in flow *changes* (L and V are deviation variables), due to the inaccuracy of valve settings. The uncertainty increases at higher frequencies, reaching a value of 100% at about $\omega = 1$ min^{-1}. The increase at high frequencies will allow for a time delay of about 1 min between L and V and the outputs y_D and x_B.

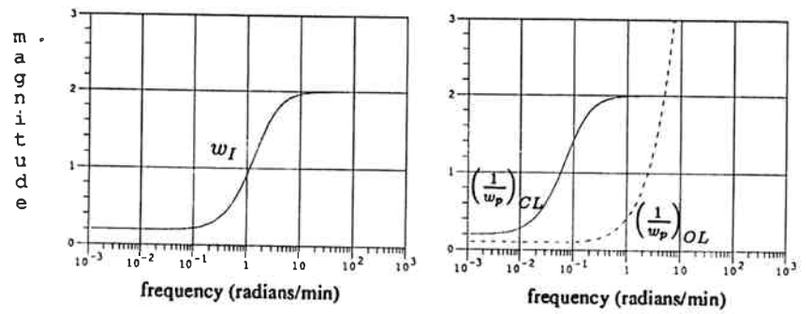

Figure 4.11: Weights for μ-analysis. a) Uncertainty weight. b) Inverse performance weights. Solid line: Closed loop, dotted line: Open loop.

Performance weights.

In the "Open Loop" test we use the following performance weight

$$w_p(s) = \frac{10}{4s+1} \tag{4.25}$$

which is shown in fig 4.11b. This weight requires less than 10% estimation error for $(1-\hat{y}_D)$ and $\hat{x}_B$ at steady-state ($\omega \leq 0.1$ min^{-1}). At higher frequencies the weight increases to one at $\omega = 2.5$ min^{-1}. This allows for an error greater than 100% at frequencies above 2.5 min^{-1}. In the "Closed Loop" test we chose a performance weight

$$w_p(s) = 5\frac{10s+1}{100s+1} \tag{4.26}$$

This implies that the deviation of $y - y_s$ should be within 20% at steady state, i.e, we tolerate a deviation of the product composition of about 0.2 mole%. Our feedback system should be effective up to about $\omega = 0.05$ min^{-1} and the amplification at high frequencies should never exceed 2. Except for the allowed steady state offset this weight is the same as the one used by Skogestad and Morari (1988).

Weights for external inputs.

The external inputs to the systems (the $\tilde{d}$'s in the block diagrams for mu-analysis) consist of setpoints, as well as ordinary disturbances and noise. They are normalized by specifying their maximum values at any frequency using weights. The maximum setpoint changes

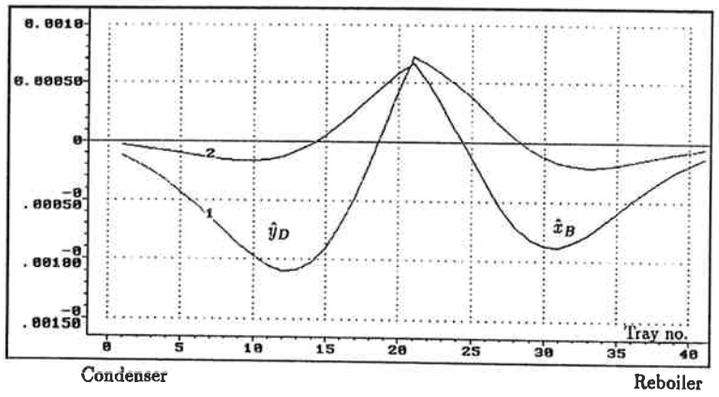

Figure 4.12: Elements in matrix K for estimation of 1) y_D, 2) x_B.

are set to 100% of x_B and $(1-y_D)$. Since the operating point is 0.01 and 0.99 this implies that the x_{Bset} may vary from 0 to 0.02, and y_{Dset} from 0.98 to 1.0. The disturbances in the feedrate F and the feed composition z_F are set to 20%, i.e. z_F may vary from 0.4 to 0.6 in mole fraction. Noise was generated by adding a constant vector of random values with normal distribution and a standard deviation of 0.2 $°C$ to all 41 temperatures. No noise is used in the mu-analysis unless otherwise stated.

4.5 Results.

4.5.1 Insights into the collinearity using PCR.

The elements in the matrix K_{PCR} for the case with 41 temperatures, are plotted in fig. 4.12. In fig. 4.13 the three largest loading vectors p are displayed. These show how the different measurements are summed up to make the latent variables (principal components). The first component is mainly due to changes in the external flows, D and B, and reflects moving the entire temperature profile up and down the column. The second component is due to changes in internal streams (with D and B constant), and reflects stretching or compressing the profile (changing the separation in the column). The third component is due to changes in the feed composition. From the figures we see that the temperatures near the product streams are weighted little compared to the ones towards the middle of the column. The reason is that the temperature variation

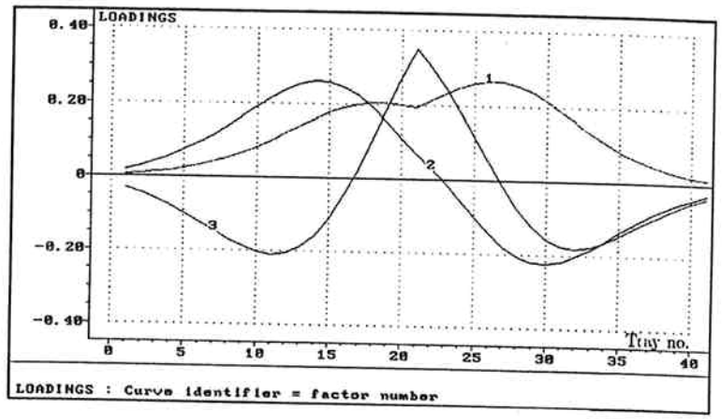

Figure 4.13: Loading plot of the first 3 principal components. Curve identifier: component number.

is small at the ends, and the measurements are therefore much more sensitive to noise. Pressure variations were not included in this study, but the temperatures near the ends of the column would be useful to compensate for such variations. The forth vector is displayed in fig. 4.14. We see that this vector contains only numerical noise, and there are, as expected, only three different directions in the temperature space when pressure is kept constant. This is also confirmed by Figures 4.15 and 4.16. They show how the different principal components account for the total variance in the calibration set both in y-space and in θ-space.

4.5.2 Number of measurements and their location.

The μ-plots in Figure 4.17 for the PCR estimator shows the effect of using varying numbers of measurements. It demonstrates that adding temperature measurements improves the estimates and the control performance. The main difference is between two and three measurements. With less than three measurements all principal components in the temperature space can not be recovered, unless they are placed towards the ends where the dimension of temperatures shrinks to one (see Figures 4.3 and 4.4). A comparison of various locations of the two temperatures are shown in the μ-plots in Figure 4.18. Without noise the best location is of course at the ends (trays 1 and 41, Case 2a in Figure 4.18a) and a perfect estimate is obtained. With noise it is better to use measurements closer to the middle of the column where the temperature changes are much larger (trays 6 and

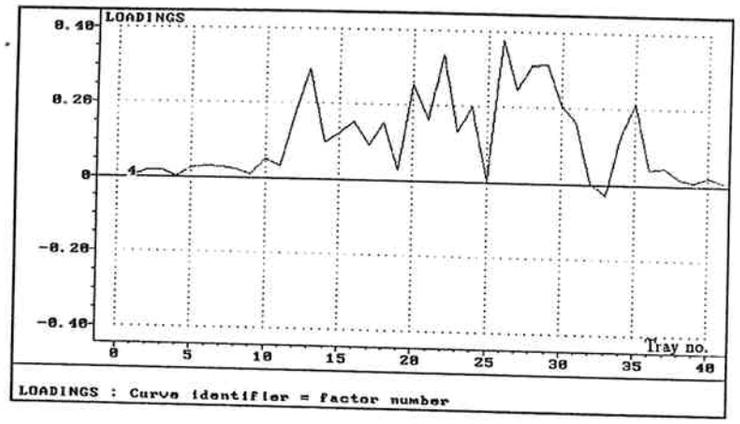

Figure 4.14: Loading plot for the fourth principal component.

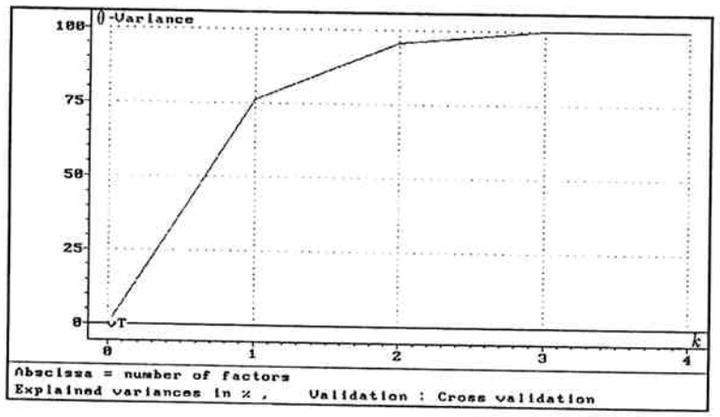

Figure 4.15: Explained Θ-variance (%). Abscissa: Number of principal components.

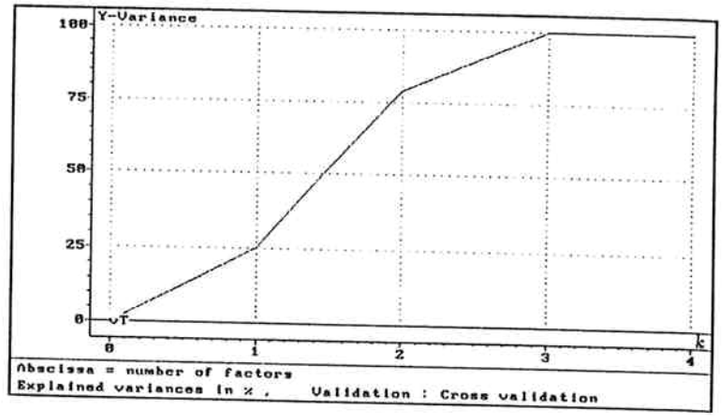

Figure 4.16: Explained Y-variance (%). Abscissa: Number of principal components.

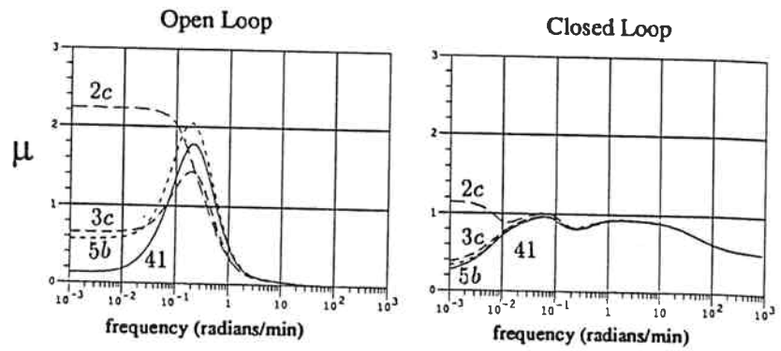

Figure 4.17: Effect on μ of number of temperatures for PCR-estimator. The temperatures in the calibration set are corrupted with 0.1 °C noise.

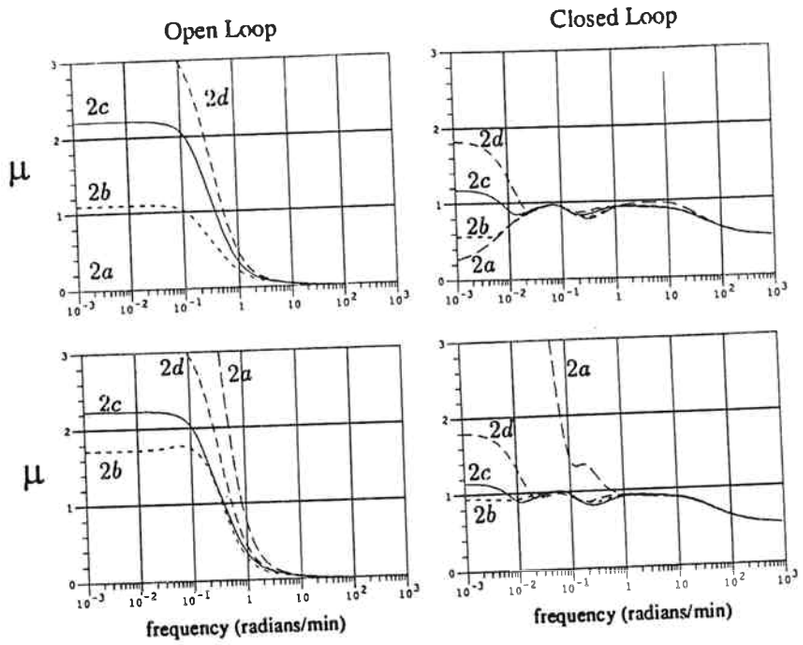

Figure 4.18: Effect on μ of noise and location for two measurements. a) PCR without noise in calibration set, b) PCR with 0.1 °C noise in calibration set.

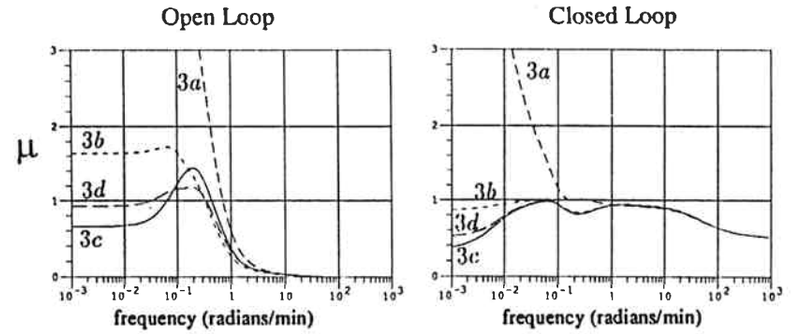

Figure 4.19: Effect on μ of location for three measurements. PCR with 0.1 °C noise in calibration set.

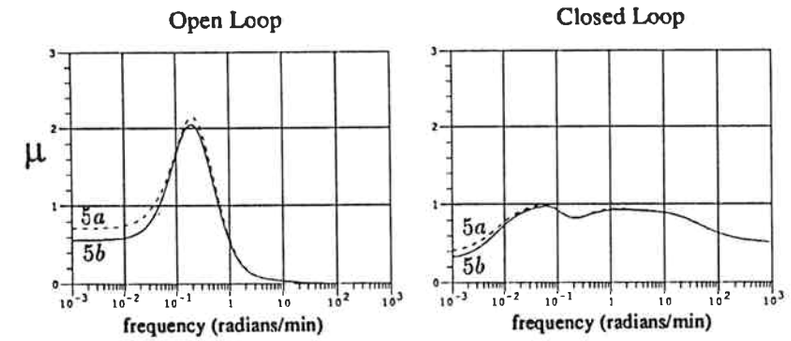

Figure 4.20: Effect on μ of location for five measurements. PCR with 0.1 °C noise in calibration set.

36, Case 2b in Figure 4.18b). The same conclusion applies to cases with three (Fig. 4.19) and five measurements (Fig. 4.20), but the location of measurements of course becomes less important as additional measurements are used, provided they are reasonably evenly spaced.

Also the Kalman filter is improved by adding measurements. This is illustrated by the μ-plots in Figure 4.21.

4.5.3 Comparison of Kalman filter and static PCR estimator.

In fig. 4.22 we compare the μ-plots of the Kalman and PCR estimators, using 41 tem-

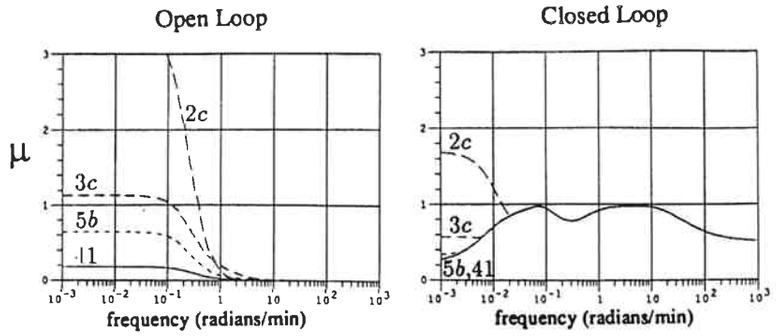

Figure 4.21: Effect on μ of number of measurements for Kalman Filter (K1). No Noise.

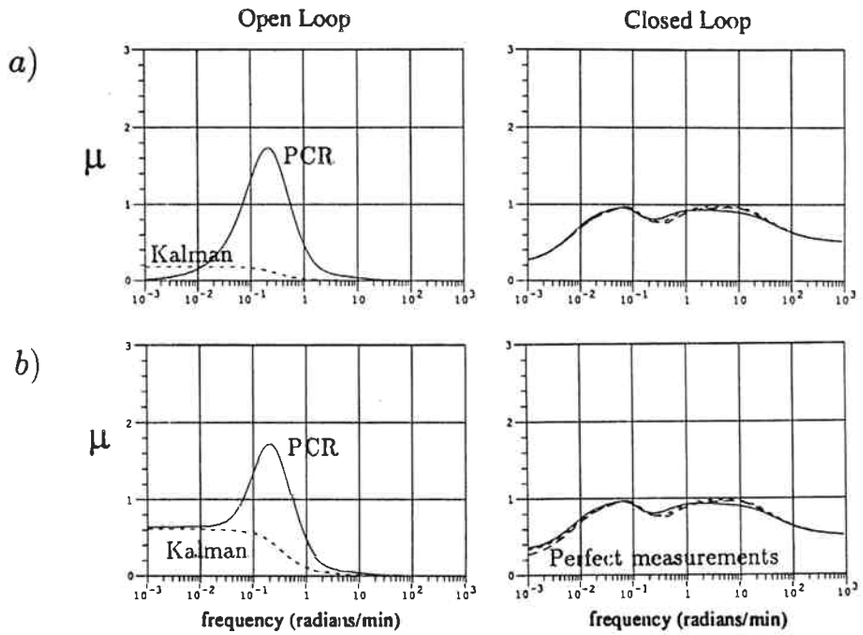

Figure 4.22: Comparison of Kalman (K1) and PCR estimator. a) without noise in μ-analysis, b) with noise.

peratures. The first thing to note is how well the simple static estimator $\hat{y} = K_{PCR}\theta$ performs. The main reason is that the dynamic responses of the temperatures θ and the compositions y are very similar. This will be the case for most distillation columns, at least for sections of the column, but may of course not be the case for other applications.

In the Open Loop analysis the Kalman filter is significantly better at higher frequencies. This is due to the dynamics included in this estimator. On the other hand, the "Closed Loop" test shows that the estimators will perform about equally well when used for feedback, and also as well as using perfect measurements. Actually, for some frequencies, the PCR estimator is even better than using perfect measurements. The reason is that the temperatures in the middle of the column generally change slightly faster than at the ends, and the steady state estimator will therefore have a small inherent "feedforward" effect. The simulation responses in Figure 4.23 confirm that the PCR-estimate is almost equal to the true value. One exception is for feed composition disturbances, where it shows a small inverse response.

4.5.4 Different Kalman filters and use of inputs in estimator.

Figure 4.24 shows μ-plots for the Kalman filters obtained using the four different levels of process noise on L and V in Table 4.2. The best Kalman filter, K1, is the one that was compared with PCR above. The remarkable thing with this best estimator is the very large assumed variance on the inputs u (L and V). In effect, this variance is so large that the transfer function from u to $\hat{y}$ in Eq.(4.10) is approximately zero, that is, the estimator does not use the information about the input signals.

The worst Kalman filter, K4, assumes disturbances (noise) of magnitude 0.1 for F and z_F, but assumes no disturbances on the inputs. This estimator performs reasonably well in the μ-test when there is no uncertainty (upper left part in Figure 4.24). (But note that disturbances on the inputs are not included in the μ-analysis.) However, it is extremely poor when input uncertainty is added (lower left).

The PCR estimator in this paper uses only temperatures, but we did also evaluate the effect of adding inputs. However, the improvement in estimator performance was very small even at steady state. Furthermore, the dynamic behaviour of the static estimator is much worse when inputs are used.

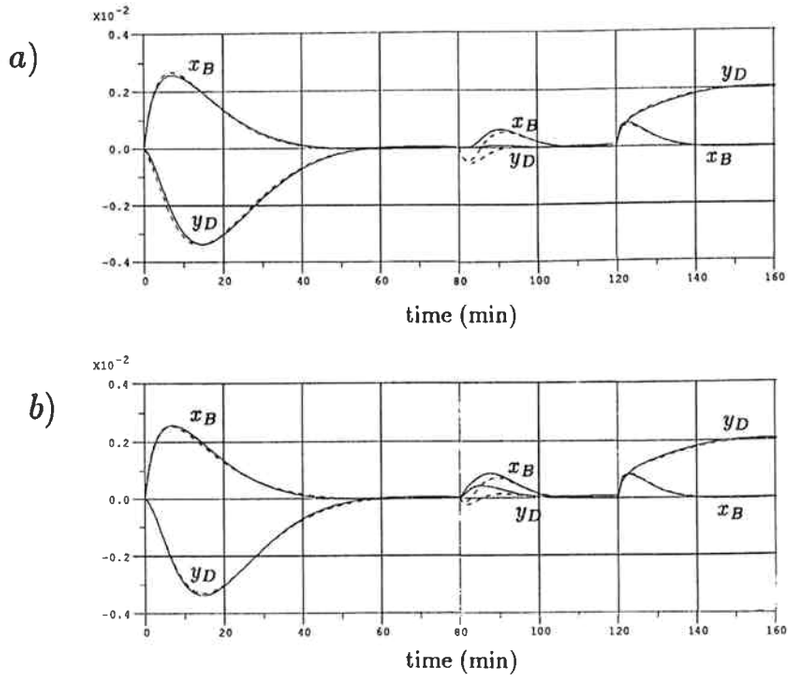

Figure 4.23: Comparison of output $y(t)$ (solid) and PCR-estimate $\hat{y}(t)$ (dotted line). Responses under feedback control are shown for a 20 % increase in feedrate at t=0, a 20 % increase in feed composition at t=80 min, and a setpoint change in y_D at t=120 min. a) y used for feedback control, b) $\hat{y}$ used for feed backcontrol.

Figure 4.24: Different Kalman filter gains (Table 4.2). Upper left: Nominal estimation error. Lower left: Robust estimation error. Upper right: Robust control error. Solid line: K4. Short dotted line: K3. Medium dotted line: K2. Long dotted line: K1.

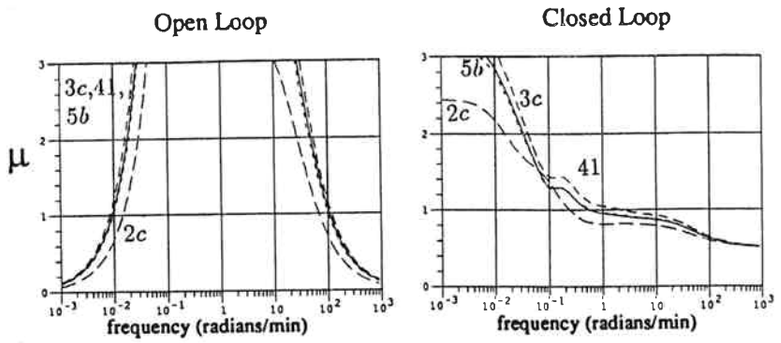

Figure 4.25: Effect of number of measurements for Brosilow Inferential Estimator. No noise.

4.5.5 Brosilow estimator.

The Brosilow inferential estimator for the system with different numbers of measurements is shown in Figure 4.25. It clearly demonstrates that the estimator as originally proposed performs poorly, and its performance does not improve with increasing number of measurements. The "Open-loop" test shows that the estimator nominally works well at very low frequencies ($\omega < 0.001$ min^{-1}). The poor dynamic performance (intermediate frequencies) is due to the fact that the estimator uses the input signals u (L and V) as shown in Eq. (4.16). The dynamic behaviour of u and the compositions y are very different and using a constant matrix $G_u - K_B F_u$ does not work well. This problem could have been corrected using a low-pass filter on the inputs with a large time constant, e.g., 194 minutes (that is, add dynamics to G_u and F_u). However, even this estimator would not perform well in practice, as the "Closed-loop" test shows that the robust performance is poor even at low frequencies. This is due to the input uncertainty, that is, the actual values of L and V are different from what the estimator thinks they are.

We therefore conclude that using the measured input signals u (which are inaccurate) does not improve the estimate. A better approach then seems to be to regard the inputs L and V as unknown disturbance together with z_f. This gives rise to the modified estimator $\hat{y} = K_{Bmod} d'$ where $d' = [L, V, z_F]^T$. This estimator performs much better as seen from curve A in Figure 4.26. The estimated values of the latent variables L, V and z_F may not be correct, but this error is not important as long as the estimate $\hat{y}$ is accurate. However, using L, V and z_F as latent variables has very poor numerical properties. For example,

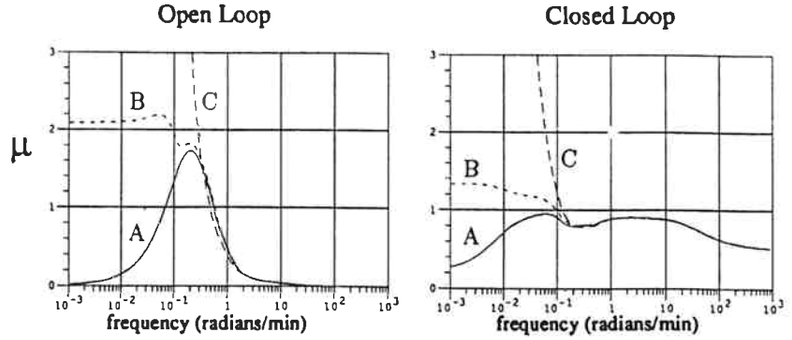

Figure 4.26: Modified Brosilow estimator based on temperatures only. 41 temperatures. A: Perfect model. B: Model rounded to 3 digits. C: Model when 1% random noise is added to process matrices.

curve C in Figure 4.26 shows the drastic deterioration in performance caused by adding 1% random error to the elements of the matrices G' and F'.

4.6 Discussion

4.6.1 Kalman filter.

Model uncertainty is not included explicitly when obtaining the Kalman filter and it may require physically unrealistic values of the noise weights, V and W, in order to obtain the best estimator when uncertainty is included. This is illustrated by the large value needed for noise (disturbances) on the inputs in order to obtain the best Kalman filter, K1. Otherwise, the Kalman Filter performed well in the μ-tests and was undoubtedly the best estimator in the open loop μ-test. The main reason is its inherent dynamics, which can track the changes in the process tightly. Furthermore, because of the weights, it is flexible, and it may be tuned to perform well for ill-conditioned plants a well. As mentioned above this is done by adding (artificial) large noise (disturbances) on the inputs to the process.

4.6.2 Brosilow estimator.

As discussed above the Brosilow Inferential estimator as originally proposed suffers from four main weaknesses:

W1. *For ill-conditioned plants (with large RGA-values) input uncertainty causes poor estimates when the estimator uses information about the manipulated inputs u.*

W2. *Even for plants which are not ill-conditioned, the dynamic behaviour of a static estimator which directly uses inputs is often poor. The reason is the dynamic "lag" which usually exists between the inputs u and the outputs y.*

W3. *It does not handle collinearity among the variables in an appropriate way.* If the number of disturbances are less than the number of measurements, like in our example column, the problem arises when there is collinearity among the disturbances. This makes the results sensitive to small numerical errors as shown above. On the other hand, if the number of disturbances is larger than the number of measurements, like in the work of Joseph and Brosilow (1978), the collinearity between temperatures creates problems. Instead of using only selected measurements as proposed by Joseph and Brosilow (1978), one should rather delete small *directions* in F_d using the singular value decomposition.

W4. *For ill-conditioned plants (with large condition numbers) the use of inputs and disturbances as latent variables is ill-conceived .*

Weaknesses W1 and W2 may be corrected using the "modified" Brosilow estimator, and also W3 may be corrected using an appropriate pseudoinverse of F_d. However, the use of secondary measurements to infer the disturbances and then estimate the primary measurements is the key idea in the Brosilow estimator, and W4 can not be corrected. To illustrate W4, consider an ill-conditioned plant, where we, in order to get a good estimate must require that:

1) The estimate of the disturbances and the inputs is very accurate (this implies that models F_u and F_d, which are used to infer the disturbances, also must be very accurate).

2) The model from disturbances and inputs to disturbances (G_d and G_u) is very accurate (it must capture the low-gain direction as well).

If the condition number of any one of these four matrices is large then the estimate may be sensitive to small numerical errors. The same applies to the modified Brosilow estimator if the matrices G' or F' are ill-conditioned. For our example column the condition numbers of G' are F' are 165 and 321. This explains the poor results in Fig.4.26. We want to stress that this sensitivity to errors in the matrix elements is different from the sensitivity to input uncertainty in W1, which is discussed in more detail below.

The estimation scheme of Brosilow is based on explaining the observations by estimating the inputs using a causal input-output model. This approach may be satisfactory in many cases, but not for ill-conditioned plants [2]. However, for such systems there may still be a rather simple direct relationship between various *dependent* variables, for example, between temperatures and composition in a distillation column, and a simple regression estimator may work well.

4.6.3 PCR estimator.

The PCR-estimator does not have the same weaknesses as the Brosilow estimator. First, the estimator used here does not use the input values, and does not suffer from uncertainty with respect to their exact value and poor dynamic performance. Secondly, and more important, its numerical properties are much better. The matrix to invert in PCR, the score matrix T in Eq. (4.22), is generally much better conditioned than F' used by the modified Brosilow estimator. For example, for our column the condition number of T is 4.7, whereas the condition number of F' is 321. To get a well-conditioned T one must ensure that excitations of the weak directions are included in the calibration set. To ensure such excitations, one should use data from the column with feedback (that is, with specified outputs), for example, by specifying the product compositions together with the feed composition in an factorial design like in Table 4.3. One should *not* use open loop data, like step responses etc., which will excite only the strong directions (The gain matrices in Brosilow's scheme will typically result from such excitations).

In an earlier study (Joseph et al., 1976) it was found that the Brosilow estimator performed better than a regression estimator. However, they used the simple least-square estimator in (4.20) which suffers from the same poor numerical properties as the Brosilow estimator.

Conceptually, it is simple to generalize the static PCR estimator to obtain a dynamic estimator. This may be done using the PCR method to derive an ARMA model relating time series data for θ and y.

Partial Least Square (PLS) estimator.

The PLS estimator is an alternative regression estimator, which also takes into account the directions in Y when finding the approximate pseudo inverse of Θ (Höskuldson 1988).

[2] The extreme of an ill-conditioned plant is a chaotic system where it is impossible to back-calculate the inputs which have caused the observed outputs

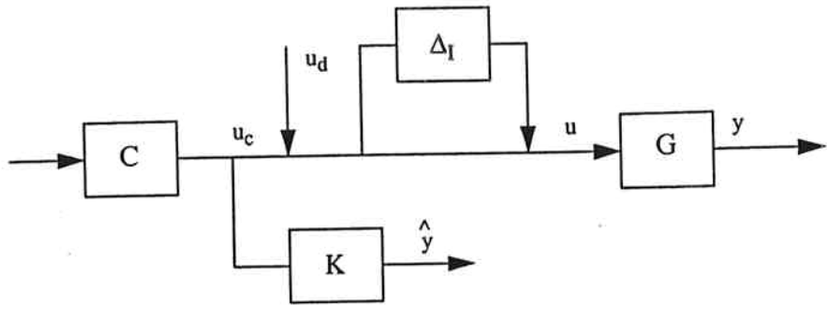

Figure 4.27: Actual input, u, may differ from value, u_c, used by the estimator because of 1) input disturbance u_d and 2) input uncertainty Δ_I.

In the PLS method this is done by considering the eigenvalues of $\Theta^T Y Y^T \Theta$ rather than of $\Theta^T \Theta$ used in PCR. This takes into account the directions in Θ which have the largest covariance with Y, and thus ensures that these directions are not deleted. For the linear distillation example studied in this paper the PCR and PLS methods gave almost identical results. However, when nonlinear data were used we found PLS to be somewhat better.

4.6.4 Use of inputs in estimator

The μ-results showed that when the inputs are used explicitly by the estimator, the Brosilow estimator and the Kalman filter (case K4) are very sensitive to input errors. By input error we mean the differences between the actual plant inputs, u, and the desired input, u_c, computed by the controller and which are used for estimation (see Figure 4.27). We consider two source of input error: 1) input disturbances, and 2) model uncertainty at the inputs. We then have

$$u = (I + \Delta_I)(u_c + u_d) \tag{4.27}$$

where u_d is the disturbance on the inputs, and Δ_I is the relative input uncertainty (see below). To understand the effect of the input error, consider the somewhat unlikely case when there are no secondary measurements, that is, $F_d(s) = F_u(s) = 0$. In this case both

the Brosilow estimator and Kalman filter become

$$\hat{y} = G_u(s) u_c \tag{4.28}$$

Assume also that there are no other disturbances (this assumption may easily be relaxed). Then the actual plant output is

$$y = G_u u \tag{4.29}$$

and the estimation error becomes

$$e_1 = y - \hat{y} = G_u(u - u_c) \tag{4.30}$$

We shall now consider separately the two sources of input error.

1. *Input disturbances.* In this case $u - u_c = u_d$ and the estimation error becomes

$$y - \hat{y} = G_u u_d \tag{4.31}$$

We note that the estimation error may be large even for small disturbances, u_d, if the elements in the matrix $G_u(j\omega)$ are large, that is, if $\bar{\sigma}(G_u(j\omega)$ is much larger than 1. This assumes that G_u has been scaled such that at any frequency expected input disturbances have magnitude 1, and the allowed estimation error has magnitude 1. In cases where $\bar{\sigma}(G_u)$ is much larger than 1, it is probably not advisable (or at least not very helpful) to use the input signals for estimation. This is typically the case for distillation columns with high-purity products. For example, in our case we have at steady-state (Skogestad and Morari, 1988)

$$G_u(0) = \begin{pmatrix} 87.8 & -86.4 \\ 108.2 & -109.6 \end{pmatrix} \tag{4.32}$$

Here the gain matrix is scaled such that the allowed estimation error is 1 in mole% (corresponds to about 100% error of the nominal impurity) and the allowed disturbances on the inputs, L and V, are equal to the feed rate (corresponds to about 30% of the nominal inputs). The largest singular value, $\bar{\sigma}(G_u(0))$, is 197.2. We conclude that the use of input signals will not be very helpful for estimation in this case. This was also confirmed by the results in this paper.

We might consider basing the estimation on, for example, D and V (DV- -configuration) rather than L and V. In this case we have $u = [DV]^T$ and the gain matrix becomes (Skogestad et al., 1988)

$$G_u^{DV}(0) = \begin{pmatrix} -87.8 & 1.4 \\ -108.2 & -1.4 \end{pmatrix} \tag{4.33}$$

This assumes disturbances on D of magnitude F. This seems large, and a value of $0.1F$ may seem more reasonable. Rescaling the gain matrix gives

$$G_u^{DV}(0) = \begin{pmatrix} -8.78 & 1.4 \\ -10.82 & -1.4 \end{pmatrix} \tag{4.34}$$

However, also in this case the elements in the matrix (and therefore also $\bar{\sigma}(G_u)$) are rather large, and the estimate will be sensitive to input errors.

2. Input uncertainty. In this case we have

$$u = (I + \Delta_I)u_c \tag{4.35}$$

where the uncertainty matrix $\Delta_I = diag\{\Delta_j\}$ is a diagonal matrix consisting of the relative input errors on each input channel j. The estimation error becomes

$$y - \hat{y} = G_u \Delta_I u_c \tag{4.36}$$

From Eq. (4.28) we have $u_c = G_u^{-1}\tilde{y}$ and we get

$$e_1 = y - \hat{y} = G_u \Delta_I G_u^{-1} \hat{y} \tag{4.37}$$

Skogestad and Morari (1987) found that the i'th diagonal element of the term $G_u \Delta_I G_u^{-1}$ is given by $\Sigma_j \lambda_{ij}(G_u)\Delta_J$ where λ_{ij} denotes the ij'th RGA-elements. Consequently, in the presence of input uncertainty, the estimation error e_1 is likely to be very large for plants with large RGA-elements. Note that this result is independent of the controller used. The model Eq. (4.32) used throughout this paper has diagonal RGA-values of 35.1, and we obtain at steady-state

$$G_u \Delta_I G_u^{-1} = \begin{pmatrix} 35.1\Delta_1 - 34.1\Delta_2 & -27.7\Delta_1 + 27.2\Delta_2 \\ 43.2\Delta_1 - 43.2\Delta_2 & -34.1\Delta_1 + 35.1\Delta_2 \end{pmatrix} \tag{4.38}$$

The elements in this matrix may be large even for very small relative input gain, Δ_j. This is consistent with the μ-analysis of the estimation error ("open-loop") where we observed very large μ-values for the Brosilow and Kalman(K4) estimators for the case with uncertainty (eg., lower left in Fig.4.24).

For plants with small RGA-elements the diagonal elements in the error term $G_u \Delta_I G_u^{-1}$ are small, but the off-diagonal elements may still be large. However, for the DV-configurations mentioned above the offdiagonal elements represent no problem. The model in (4.34) has diagonal RGA-values of 0.45 and we obtain

$$G_u^{DV} \Delta_I G_u^{DV^{-1}} = \begin{pmatrix} 0.45\Delta_1 + 0.55\Delta_2 & 0.45\Delta_1 + 0.45\Delta_2 \\ 0.55\Delta_1 + 0.55\Delta_2 & 0.55\Delta_1 + 0.45\Delta_2 \end{pmatrix} \tag{4.39}$$

All elements in this matrix are small. This implies that an estimator which uses information about D and V will *not* be sensitive to input uncertainty. However, as noted above it may still be sensitive to input disturbances. Furthermore, we found for the PCR estimator, that adding input information did not improve the estimate significantly even the case of no input error (caused by disturbances or uncertainty). The reason is that the temperature measurements contain most of the relevant information.

When secondary measurements, θ, are used by the estimator, then some of the input error may be detected and corrected for. Nevertheless, the results above demonstrate that the estimator should *not* use information about the input signals for plants where either 1) G_u (when appropriately scaled) contains large elements, or 2) G_u has large RGA-elements. Both these cases are often encountered for ill-conditioned plants. Note that the RGA is independent of scaling.

The conclusion for our distillation column is to base the estimate on temperature measurements only. Input information does not improve the estimate because of 1) sensitivity to input error, 2) poor dynamic response when used in a static estimator, and 3) the fact that the temperatures contain so much information that the estimate is not improved significantly (even if we disregard the first two items).

4.6.5 μ-analysis of estimators

The structured singular value, μ is a powerful tool for comparing multivariable linear systems with unknown disturbances and uncertainty, without having to perform a large number of simulations. Since μ is a worst case measure, this tool discovers explicitly the weak spots in a system. For example, it would have been much more difficult to discover the estimators' sensitivity to input uncertainty from simulations. However, the test requires additional modelling effort to capture the uncertainty in an adequate way.

While using the μ analysis we encountered problems with how to include measurement noise. Modelling it as independent disturbances would give a worst-case combination which would be extremely unlikely to occur when there are many temperatures. Therefore, in the μ-analysis we added the noise as $n = kn_0$, where k is a frequency-dependent constant to be varied in the μ-analysis, but where n_0 is a constant random vector. This approach works well when comparing estimators with the same location and number of measurements. However, in other cases the specific value of the random numbers in the noise vector n_0 may be important and may bias the μ-values. When comparing various

PCR-estimators we therefore did not include noise in the μ-analysis. However, here we included noise on the calibration sets.

4.6.6 Nonlinearity

All models used in this paper are linear. This simplifies the problem and is necessary for using the μ-analysis. But distillation columns are known to be very nonlinear, so the effect of nonlinearity should be taken into consideration. Nevertheless, in general a system that does not perform well in the linear case, will not perform well in the nonlinear case, and a linear study is therefore a good first step in a performance evaluation.

The Kalman Filter may be extended to the nonlinear case using the so-called Extended Kalman Filter, where the process matrices and the gains are updated on-line. For distillation columns this may give a heavy computer load. For the PCR/PLS estimator the use of additional principal components may be used to eliminate some of the nonlinearity.

For distillation columns an alternative way to counteract nonlinearity is to use logarithmic transformations of the compositions (Joseph and Broslilow, 1978, Skogestad and Morari, 1988). This approach may be used for all estimators. In another paper by the authors, the questions of nonlinearity and multicomponent mixtures will be discussed in detail.

4.6.7 Obtaining and implementing the estimators

Both the Kalman filter and the Brosilow estimator require a linear open-loop model. On the other hand, the PCR approach only deals with the data. This is an advantage, especially when experimental data are used, but also when we do have a good model, as in this paper, since we save a significant effort in obtaining the linear model matrices.

To obtain the Kalman filter one must specify weighting matrices for noise and disturbances. These may be difficult to determine *a priori*, especially since the best value of these weights may not be physically meaningful. The Brosilow estimator has the advantage of having essentially no tuning parameters, but this makes it inflexible, and it does not work for ill- conditioned plants. Although not discussed in this paper, the PCR/PLS estimator depends strongly on the scaling of the variables. These scalings are then effective tuning parameters, which are used primarily to reflect the measurement noise. In this paper no variable scaling was applied.

As for implementation, the static Brosilow and PCR estimators are of course much simpler than the dynamic Kalman filter. For all estimators it is necessary to have some scheme for dealing with measurement failures, that is, to detect and correct outliers.

Pressure variations were not included in this study. Pressure compensation is easily included in the PCR estimator if different pressure levels and pressure drops are included in the calibration data set.

4.7 Conclusions

1. With the Kalman and PCR estimators, the estimate is improved by adding temperature measurements. With more than three temperatures the improvement for our example column is mainly to reduce the effect of measurement noise. The Brosilow estimator does not handle collinearity well and the estimate is not improved by adding temperatures. In general, one should not use few measurements (that is, delete measurements), but rather use only a few *combined* measurements (in the dominant directions of the measurement space).

2. From a theoretical point of view it is obvious that one may always improve the estimate by "appropriate" use of additional information (measurements). However, in some cases the usefulness of the additional information may be minimal (see use of inputs below). In other cases the improvement of the estimate must be traded off against the cost of obtaining the measurements and the increased chance of failures. Therefore, in practice one may not always want to use additional measurements.

3. For plants with large elements in the appropriately scaled gain matrix, G_u, the presence of *input disturbances* implies that the use of input signals does *not* improve the estimate. This will be the case for most high-purity distillation columns.

4. For ill-conditioned plants with large RGA-elements for G_u, the presence of *input uncertainty* implies that the use of input signals does *not* improve the estimate. This was illustrated for our example column by the Kalman filter where the best tuning corresponds to not using information about the input flows.

5. The Brosilow estimator uses the inputs directly and the estimate may be very sensitive small errors in input measurements. In the modified Brosilow estimator,

introduced in this paper, the inputs are regarded as disturbances and this sensitivity is avoided. However, the estimate remains sensitive to small model errors if the condition number is large.

6. In the case of perfect models the modified Brosilow estimator and the (linear) PCR estimator are equivalent. This is quite obvious since both minimize the 2-norm of the estimation error. However, for ill-conditioned plants, PCR is better behaved numerically and is less sensitive to model errors.

7. When the dynamic response of the process outputs and the secondary measurements are similar, a static estimator may be sufficient. This is the case for our distillation example when inputs are *not* used.

8. For our distillation example, the PCR and Kalman estimators were almost identical in the closed-loop μ-test. The Kalman filter is more difficult to implement, requires more computer time, and needs initialization of the states. Thus the much simpler static PCR estimator is preferable.

9. The PCR and PLS estimators gave very similar results for our linear distillation example.

10. The exact location of the temperature measurements is important when few measurements are used, but is less critical for our example when we have about four or more measurements. 10. It is important to check the performance of an estimator both in "open loop" (estimation error) and in "closed loop" (control error). Some errors in the "open loop" estimation may have only minor influence in closed loop. One disadvantage with the closed loop test is that it depends heavily on the controller chosen.

11. Although the μ-analysis has some difficulties of representing noise, it was found to be most suitable for studying the performance of the estimators for this ill-conditioned plant.

In conclusion, we believe that our study presents a number of results which may prove useful in practical control of distillation columns. Temperature measurements are reliable and without delay, and the need for on-line GC measurements, which are very unreliable, may be eliminated. However, a less frequent update based on, for example, using off-line

GC may be needed. We also believe that our comparisons of various estimators, and the analysis of sensitivity to input error, are of interest from a general point of view.

NOMENCLATURE.

d - disturbances
D - distillate flow rate
$\tilde{d}$ - external inputs in μ-analysis
F - feed flow rate
F_i ,F' - Gain matrixes from inputs to secondary measurements (temperatures)
G_i, G' - Gain matrixes from inputs to primary outputs.
K - estimator matrix
K_f - Kalman filter gain
L - reflux flow rate
N - number of theoretical trays
N_F - location of feed tray
p - loading vector (direction of principal component) or no. of y-variables
PCR - Principal Component Regression.
q - no. of θ-varibles
q_F - fraction liquid inn feed
t - principal component (score), latent variable
T - matrix of scores
u - manipulated inputs $(= (L, V)^T)$
v - process noise (disturbance)
$\mathcal{V}$ - process noise covariance matrix.
V - boilup rate from reboiler
w - measurement noise
w_i - input uncertainty weight
w_p - performance weight
$\mathcal{W}$ - measurement noise covariance matrix.
x_B - mole fraction of light component in bottom product
y - output vector $= (y_D, x_B)^T$
y_D - mole fraction of light component in distillate
z_F - mole fraction of light component in feed

Greek symbols

α - relative volatility

Δ - uncertainty block

$\gamma(A)$ - condition number of matrix A

μ - Structural Singular Value

ω - frequency (min^{-1})

$\sigma_i(A)$ - The i'th largest singular value of matrix A

θ - secondary measurements (temperature vector)

$\tilde{\theta}$ - vector of all available information

Θ - data matrix of θ

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Chapter 5

Estimation of Product Compositions from Temperature Measurements by Multivariate Calibration

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Abstract

The paper addresses the use of temperature measurements to estimate product compositions in distillation columns. A simple linear multivariate calibration procedure based on steady state data is used, which requires minimal modelling effort. It is found that these PCR– and PLS–estimators perform well, even for multicomponent mixtures, pressure variations, and nonlineartity caused by changes in operating conditions. The use of weighting functions, additional factors and logarithmic transformations improve the estimates and counteract nonlinearities, provided there is not too much noise on the temperatures. The estimators employed in the paper use temperatures on all trays, but only 3–7 temperatures are necessary. The calibration coefficients from the original full set of temperatures may then provide a basis for the measurement selection.

5.1 Introduction.

Reliable and accurate measurement of product compositions is one of the main difficulties in distillation column control. Most product analyzers, like gas chromatographs, suffer from large measurement delays and high investments and maintenance costs. The overall measurement delay is typically 10 to 20 minutes. This imposes severe limitations on achievable control performance. However, the reliability of the analyzers is perhaps their weakest point, and this also results in high maintenance costs in terms of manpower and expensive back up systems. One employee per every three GC analyzers is common in industry. The most popular alternative to analyzers is single temperature control, i.e., control of a given tray temperature. Temperature measurements are reliable and inexpensive, and have negligible measurement delays. However, they are not accurate indicators of product composition. Nevertheless, in most cases temperature control is preferred. For example, Kister (1990) recommends using temperature control unless the difference in boiling point between the key components is very small, or there are substantial economical benefits in keeping tight control of the product compositions.

This paper addresses two-product columns where we make a split between two defined key components, denoted the light (L) and heavy (H) key component. We can make two independent specifications to define the split between these components. The distribution of the remaining components, denoted the off-key or non-key (N) components, may not be specified. In this paper the specifications are chosen as the product mole fractions, y'_D and x'_B, of light component on a pseudo binary basis.

Problems with single temperature control. Figure 5.1 displays typical steady state profiles for the binary example column[1]. For this binary mixture at constant pressure, the temperature at the column end is an exact indicator of composition. However, as seen from Figure 5.1 the temperature variation is very small at the top and at the bottom of the column and may be difficult to distinguish from measurement noise. Therefore, temperatures further removed from the end are preferred (Nisenfeld and Seeman, 1980). However, the use of a single temperature to indicate product composition is generally not reliable because of the following:

- Composition changes. Even for binary mixture the relationship between a temperature inside the column and a product composition, depends on the feed composition, and also on the product composition at the other end of the column.

[1]The column is described in section 5.2.1

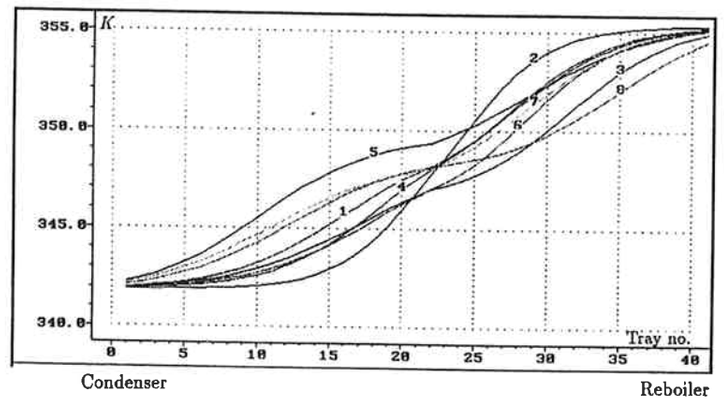

Figure 5.1: Steady state profiles of the example column. Binary mixture.

- Off-key components. For multicomponent mixtures the presence of off-key components implies that even at the column ends temperature is not an exact indicator of composition. The effect of variations in off-key components is largest near the feed and at the column ends.

- The measurement device. 1) Random noise associated with the measurement and data treatment device. This high frequency noise will have the same magnitude on all trays. 2) Low-frequency measurement offsets, for example, due to fouling or changes in the ice-point temperature compensation.

- Temperature variations due to flow pulses and improper mixing on the trays. These variations have a peak at intermediate frequencies and are largest in column sections with large temperature gradients.

- Pressure changes. 1) Changes in total pressure which have a similar effect on all temperatures. 2) Changes in pressure drop due to changes in throughput, which yields the largest pressure change near the bottom. Varying liquid holdups and tray performances may give local pressure variations as well.

Some measures may be taken to counteract these problems. The high frequency noise may easily be filtered. Pressure variations may be compensated using pressure measure-

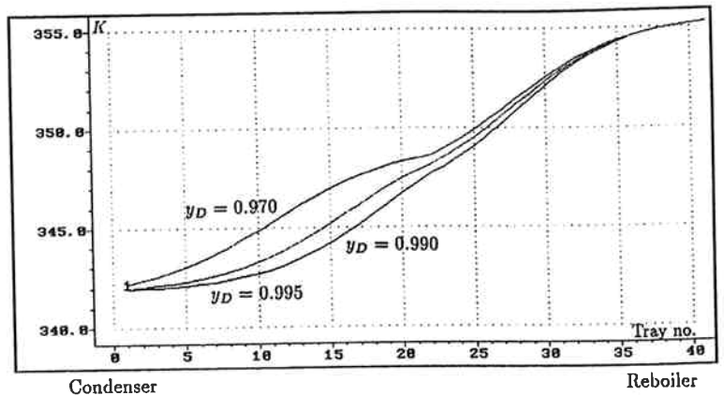

Figure 5.2: Effect of changes in top composition on the temperature profile. The feed and bottom compositions are constant.

ments, or using differential temperatures. The effect of non-key components may be reduced by locating the temperature measurement in regions of the column where their composition is nearly constant (Rademaker et.al., 1975).

However, some of these problems may not be corrected. In particular, keeping a temperature constant on a tray some distance away will not keep the product composition constant. For example, consider Figure 5.2 where it is shown that the temperatures in the lower part of the column are affected by changes in top composition, and Figure 5.3 where it is shown how the temperatures are affected by different feed compositions.

Multiple temperatures. One solution to these problems is to use multiple temperature measurements to infer the product composition. There has recently been reports from industry on sucessful implementations of somewhat *ad hoc* approaches. Whitehead and Parnis (1987) used a weighted temperature average of differential temperatures on a C_2–splitter. Bozenhardt (1988) used multiple temperatures to track the maximum temperature difference between two trays in an alcohol/water/ether column. He found the position of this maximum difference to be strongly correlated to the product composition.

A more rigorous approach is to use a temperature–based composition estimator. In another paper (Mejdell and Skogestad, 1990) we compared rigorously three different estimators using *linear* data for the binary example column. These estimators were the

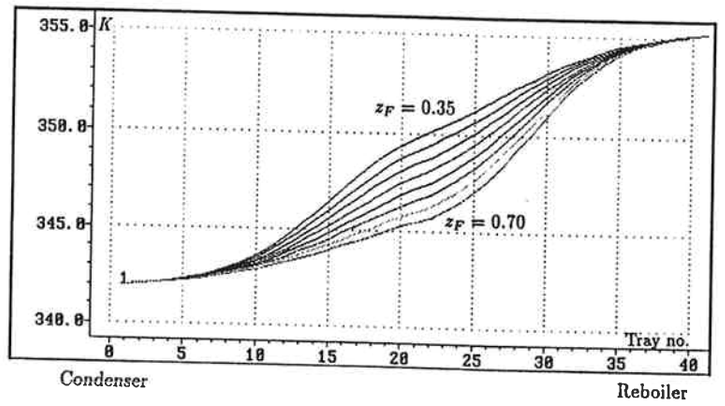

Figure 5.3: Effect of changes in feed composition on temperature profile. Top and bottom compositions are constant.

dynamic Kalman-Bucky filter (Kalman and Bucy, 1961), the static Brosilow Inferential Estimator (Weber and Brosilow, 1972, Joseph and Brosilow, 1978), and the static Principal Component Regression Estimator. It was found that for feedback control the static PCR estimator performed almost as well as the Kalman filter. The reason is that the temperatures and the compositions have similar dynamic responses. The Brosilow Estimator was very sensitive to model error for this ill-conditioned plant with large RGA-values. Mejdell and Skogestad (1990) therefore recommended using the simple regression estimator, which is obtained simply by considering corresponding values of temperatures and composition. Such data sets are most easily obtained from simulations.

In this paper we consider some additional aspects of using regression estimators for composition estimation, including

- nonlinearities in the column
- pressure variations
- multicomponent mixtures
- measurement noise.

We discuss different ways of handling these problems, such as variable transformations and scaling.

In the paper temperature measurements on all trays are used. This is not because it is strictly necessary, but to emphasize that all available measurements should be used, and to exclude the influence of measurement selection, which otherwise would bias the results.

5.2 Problem definition.

The following problem is treated in this paper: Given the temperatures on all trays in a distillation column, find a good *static* estimator for the product compositions. The example column described below is used to illustrate the main issues.

5.2.1 Example column.

The column has 40 theoretical stages (including the reboiler), and a total condenser. The feed stream enters the column at stage 20 as saturated liquid. Two cases are considered:

1. Binary mixture with constant relative volatility of 1.5.
2. Multicomponent mixture consisting of one heavy and one light non-key in addition to the binary components in case 1.

The column in case 1 is "column A" (Skogestad and Morari, 1988b), which is the same example as used by Mejdell and Skogestad (1990). Data for the column and for the mixtures are given in Table 5.1. The difference in boiling point between the two pure key components is only 13 °C. This is approximately the lower limit for what is usually recommended when using single temperature control (Riggs, 1990).

5.2.2 The estimation problem.

Consider the case with binary mixture, constant pressure and feed and reflux as saturated liquid. Then specifying different values of feed composition z_F, distillate composition y_D, and bottom product x_B, yields unique steady state profiles of the 41 temperatures θ. This may be expressed as

$$\theta^{41\times1} = f(z_F, y_D, x_B) \tag{5.1}$$

We want to find the inverse relation

$$\hat{y}^{2\times1} = \begin{pmatrix} \hat{y}_D \\ \hat{x}_B \end{pmatrix} = g(\theta^{41\times1}) \tag{5.2}$$

A. Binary mixture:

i	comp	z_F	y_D	x_B	$\alpha_{i,i+1}$	T^b (K)	Antoine parameters A	B	C
1	LK	0.500	0.99	0.01	1.5	341.9	15.83660	2697.55	-48.78
2	HK	0.500	0.01	0.99		355.4	15.43113	2697.55	-48.78

B. Multicomponent mixture:

i	comp	z_F	y_D	x_B	$\alpha_{i,i+1}$	T^b (K)	A	B	C
1	LNK	0.050	0.125	0.000	2.0	321.4	16.52975	2697.55	-48.78
2	LK	0.350	0.866	0.006	1.5	341.9	15.83660	2697.55	-48.78
3	HK	0.350	0.009	0.577	2.0	355.4	15.43113	2697.55	-48.78
4	HNK	0.250	0.000	0.417		370.1	14.73799	2697.55	-48.78

- $lnP(mmHg) = A - B/(\theta(K) + C)$
- Feed is saturated liquid.
- Constant molar flows.
- Ideal VLE using Raoults law
- Constant pressure, 1 atm.
- $N = 40, N_F = 21$ (theoretical trays)
- Holdup on all trays; $M_i/F = 0.5$ min
- Flow dynamics are neglected.

Table 5.1: Data for distillation column example.

The simplified linear estimator used in this paper may be written

$$\hat{y} = K\theta \tag{5.3}$$

where the matrix K is of dimension 2×41. The problem is to find optimal values of these 82 parameters. These parameters can not be determined independently because 1) the temperatures are not independent, and 2) there is not enough degrees of freedom in the excitations. The first fact is illustrated by Figure 5.1 where we see that temperatures close to each other changes in nearly the same way. From Equation (5.1) we see that there are only three degrees of freedom in the excitations, and the temperatures have only three different ways to vary. However, note that the number of directions in the *linear* temperature space may be larger than three if large perturbations are used in z_F, y_D and x_B. Pressure variations and off-key components also increase the degrees of freedom but they are for the moment assumed to be constant.

The estimation problem may be divided in two steps:

1. Data reduction of the temperatures into k latent variables t (also denoted factors):

$$t^{k\times 1} = p(\theta^{41\times 1}) \tag{5.4}$$

2. Obtain estimator by finding a relationship between the latent variables and the product composition.

$$\begin{pmatrix} \hat{y}_D \\ \hat{x}_B \end{pmatrix} = g(t^{k\times 1}) \tag{5.5}$$

The key question is now how to find suitable latent variables, in order to make the second regression step easy. Preferably the latent variables should be independent, and they should contain all the original information relevant for estimating the compositions.

- The simplest is to delete measurements and select only a few which are mutually independent. Then the problem of optimal measurement selection becomes a key issue. A lot of articles have been published on this subject, for example, Joseph and Brosilow (1978), Morari and Stephanopoulos (1980), and Moore (1986).

- Use unknown disturbances as latent variables. This procedure has been proposed by Brosilow and co-workers and employed in their inferential control, e.g. Weber and Brosilow (1972) and Joseph and Brosilow (1978).

- Use some geometric shape factors of the temperature profile as latent variables. This idea is used by Gilles and Retzbach (1980) and later by Marquardt (1988). Here the first factor is the location of the steepest temperature gradient.

- Use the principal components (PCR method) or the partial least square factors (PLS method) as latent variables. These methods have been introduced for distillation columns by Mejdell and Skogestad (1990), and are further outlined in the next section.

The simplest of the above methods is of course to reduce the number of measurements. However, this is not optimal, because additional measurements will

- improve the estimate because they contain more independent information (at least for few measurements)

- reduce the effect of measurement noise

- make the estimator less sensitive to measurement selection and changes in operating conditions

- better capture the effect of nonlinearities.

We have briefly investigated Marquard's method and found it to perform very well with perfect measurements, but it was sensitive to measurement noise for our column. It might perform better for distillation columns with sharp profiles, for which it was originally developed.

The Brosilow estimator was studied in detail by Mejdell and Skogestad (1990). We found that it performed poorly for the binary distillation example. The reason is that for ill-conditioned plants, like distillation columns, the estimate is very sensitive to small errors. This sensitivity has indeed been pointed out also by Brosilow and co-workers.

Mejdell and Skogestad (1990) studied the static PCR estimator for the example column and found that it performed almost as well as an optimally tuned Kalman filter. In this paper we shall use the static regression estimators, PLS and PCR.

5.2.3 Use of transformed variables.

The composition and temperature profiles are nonlinear functions of the operating variables. One way to deal with nonlinearity is to find other variables (factors) which can

capture the nonlinearity. The Marquard method is one such method. A simpler method is to use nonlinear transformations on each variable. Logarithmic transformation of the product compositions has been proposed by several authors (eg., Joseph et al., 1976) as an effective way to linearize the dynamic and static *response* (with L, V, F, z_F etc. as independent variables). For binary mixtures

$$Y_D = \ln(1 - y_D); \quad X_B = \ln x_B \tag{5.6}$$

These transformations apply also for multicomponent mixtures if pseudobinary compositions are used. The composition *profile* (with tray number as an independent variable) may also be linearized using similar transformations. Ryskamp (1981) plotted the compositions on a probability scale. It is also common to use the logarithm of the separation parameter (eg., PROCESS, 1981)

$$X = ln\frac{x_L}{x_H}, \tag{5.7}$$

Skogestad and Morari (1988a) showed that this transformation also linearizes the dynamic response. Note that since most columns have $y_D = x_{DL} \approx 1$ and $(1 - x_B) = x_{BH} \approx 1$, (5.6) may be viewed as a special case of (5.7).

Temperature is often a nearly linear function of composition. We therefore propose to use the following transformation to linearize the temperature response and profile

$$L_T = \ln(\frac{\theta - T_L^b}{T_H^b - \theta}) \tag{5.8}$$

Here T_L^b and T_H^b are the boiling temperatures of pure light and heavy components, respectively. For our example column this results in a nearly linear profile as shown in Figure 5.4 (compare with the unscales profiles in Figure 5.1). Column with pinch zones around the feed will not have a linear profile.

Instead of using boiling temperatures, one may use the transformation

$$L_\theta = \ln(\frac{\theta - \theta_L}{\theta_H - \theta}) \tag{5.9}$$

where θ_L and θ_H is some *reference temperature* at the top and the bottom of the column, respectively. For binary mixtures, one may use the temperature at the column end, which is very close to the boiling temperature. For multicomponent mixtures, one must select the reference temperature at a location some distance away from the ends where the effect of changes in operating conditions and off-key components is less. To avoid taking logarithms of negative numbers, the temperatures between the reference locations and

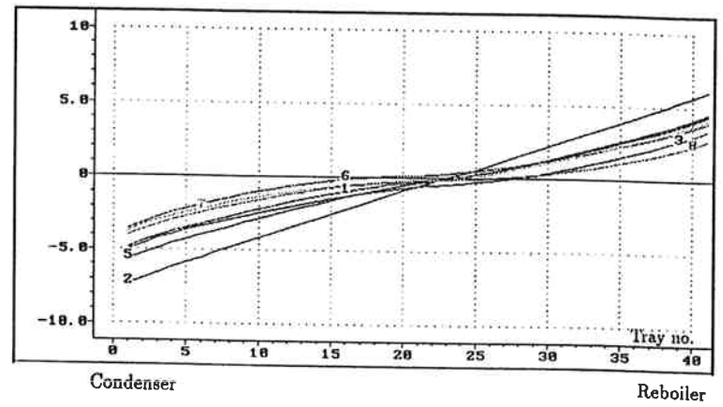

Figure 5.4: Temperature profiles in terms of logarithmic transformed temperatures, L_T.

column ends must be treated separately, for instance by using the absolute value of the temperature differences in Eq. (5.9). To avoid large effects of noise on the temperatures closest to the reference temperatures one should also specify a lower permitted limit on the difference temperatures in Eq.(5.8) and Eq. (5.9).

Using reference temperatures instead of boiling point temperatures also provides pressure compensation of the temperature measurements.

5.2.4 Multicomponent mixture.

The multicomponent mixture is the originally binary mixture extended with one light nonkey (LNK) and one heavy nonkey (HNK) component (See Table 5.1). The control objective for the separation is still the split with respect to the key components. Let x' denotes the pseudo-binary molefraction (based on key components) of light key component, i.e.

$$x' = \frac{x_L}{x_L + x_H} \tag{5.10}$$

The product specification for both the binary and multicomponent case is $y'_D = 0.99$ and $x'_B = 0.01$.

The composition profile for the multicomponent mixture at the nominal operating point is displayed in Figure 5.5. The off-key components are almost constant in the

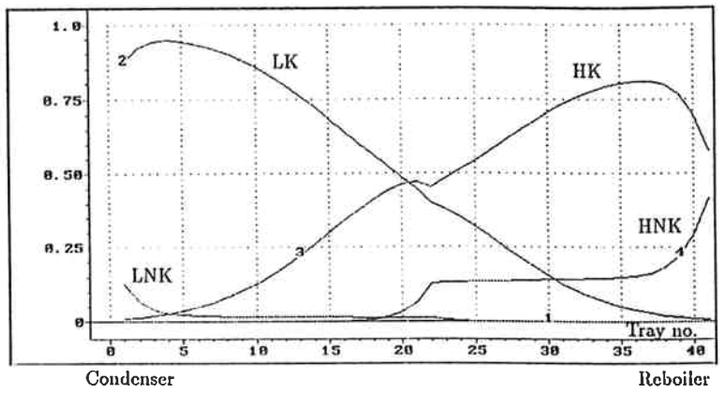

Figure 5.5: Concentration profiles of the multicomponent mixture.

column except at the column ends and around the feed tray. The composition profile on a pseudobinary basis, x', is compared with that of the binary example column, x, in Figure 5.6, and the corresponding temperature profiles are shown in Figure 5.7. The concentration profiles are almost identical, whereas the temperature profiles are quite different.

5.2.5 Calibration set for PCR and PLS.

The calibration set used in the paper consists of 32 different simulation runs. The outputs x_B and y_D and the feed composition z_F (disturbance) were specified, and the corresponding steady-state temperature profiles obtained using a nonlinear column model. The 32 values are listed in Table 5.2. The data were spread with equal distances around z_F, x_B and y_D. The first run in the left column is the nominal operating point, the other 15 runs were randomly chosen. The 16 runs in the right column were selected by a two composite design in four levels. These 32 runs correspond to maximum variations in column end temperatures of about 0.4 °C and of interior temperatures of about 5 °C.

Different versions of the 32 calibration set was made, which included

- Total pressure variations of ± 0.1 atm spread randomly on the various runs.
- Normal distributed random noise of magnitudes 0.1 or 0.2 °C on all temperatures.

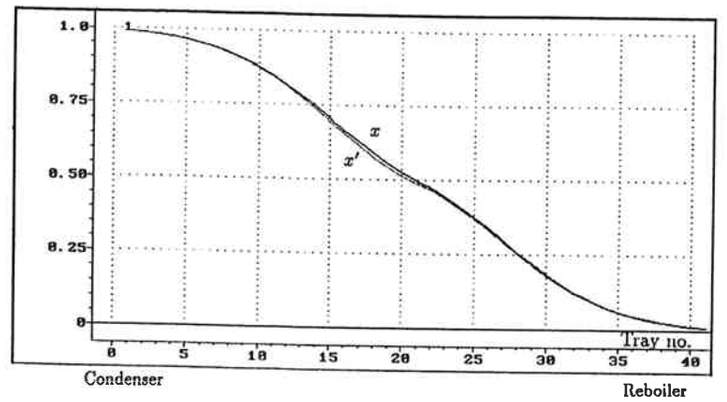

Figure 5.6: Concentration profiles for binary molfraction (x) and multicomponent pseudo-binary molfraction (x').

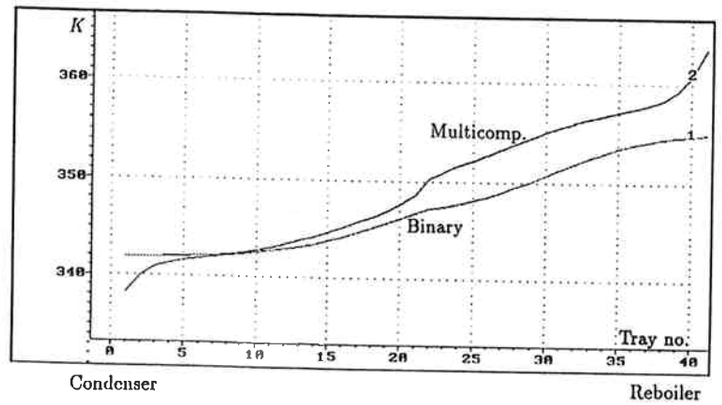

Figure 5.7: Temperature profiles for the binary and multicomponent cases.

z_F	y_D	x_B	z_F	y_D	x_B
0.5000	0.99000	0.01000	0.4000	0.97000	0.03000
0.5375	0.99130	0.02620	0.4000	0.97000	0.00333
0.4250	0.97380	0.01510	0.4000	0.99667	0.03000
0.5250	0.97000	0.01320	0.4000	0.99667	0.00333
0.4125	0.98010	0.00580	0.6000	0.97000	0.03000
0.6000	0.98490	0.00440	0.6000	0.97000	0.00333
0.5125	0.99420	0.00660	0.6000	0.99667	0.03000
0.5500	0.98270	0.00760	0.6000	0.99667	0.00333
0.4875	0.99620	0.01890	0.4500	0.98268	0.01732
0.4750	0.99560	0.00870	0.4500	0.98268	0.00577
0.5625	0.99340	0.01150	0.4500	0.99423	0.01732
0.4625	0.97720	0.03000	0.4500	0.99423	0.00577
0.4375	0.99500	0.00380	0.5500	0.98268	0.01732
0.4500	0.99240	0.01730	0.5500	0.98268	0.00577
0.5750	0.98680	0.02280	0.5500	0.99423	0.01732
0.5875	0.98850	0.00500	0.5500	0.99423	0.00577

Table 5.2: Specifications used in simulations to obtain static temperature profiles. P = 1.0 atm.

- Non-key components. The pseudobinary compositions were as in the binary case (Table 5.2), but in addition the feed molefraction of light non-key component were varied between 0.025 and 0.075, and of heavy non-key between 0.15 and 0.35. All temperatures were rounded to one decimal, which may be viewed as a (coloured) noise source.

5.2.6 Evaluation criteria.

The main criterion used to evaluate the performance of the estimators is the Mean Square Error of Prediction (MSEP), which is a measure of the expected error of *future* predictions. An estimate of MSEP was performed by a cross validation procedure as follows: The 32 calibration runs were divided into seven groups. Then the calibration procedure (i.e., finding the estimator K) was performed seven times, each time with six groups used for calibration and one for testing. The mean square error of all test predictions was then obtained from

$$MSEP(k) = \frac{1}{32}\sum_{i=1}^{32}(\hat{y}_i(k) - y_i)^2 \tag{5.11}$$

Here k is the number of factors (or principal components) used in the calibration, and y_i is y_D or x_B for the i'th test run. MSEP will generally *not* go to zero when the number of factors increases, since the test runs are independent from the ones used in the calibration. Rather, MSEP will increase when factors containing only noise are included.

We then compute the Explained Prediction Variance in %

$$EPV(k) = 100(1 - \frac{MSEP(k)}{MSEP(0)}) \tag{5.12}$$

MSEP(0) is approximately the variance in the calibration data.

5.3 Data treatment and multivariate regression.

We want to estimate p outputs (y) from q known variables (θ). Multivariate regression is a linear statistical technique for obtaining the matrix K in

$$\hat{y} = K\theta \tag{5.13}$$

Both vectors y and θ are centred (deviation variables) so there is no constant term. Obtain a "training set" consisting of n calibration runs of corresponding values of y and θ, and place these as rows in the matrices $Y^{n\times p}$ and $\Theta^{n\times q}$. We have the desired relation

$$Y = \Theta K^T \tag{5.14}$$

The general least square solution for K is (Strang, 1981, p. 139)

$$K^T = \Theta^{\dagger} Y. \tag{5.15}$$

In addition to minimizing $(y - \hat{y})^2$ this solution minimizes the norm of K. The pseudoinverse $\Theta^{\dagger}$ is most easily obtained using the SVD of Θ.

5.3.1 Singular Value Decomposition (SVD).

The SVD of Θ may be written

$$\Theta = U\Sigma V^T \tag{5.16}$$

or as a sum of m rank 1 – matrices (of decreasing importance)

$$\Theta = u_1\sigma_1 v_1^T + u_2\sigma_2 v_2^T + \cdots + u_m\sigma_m v_m^T \tag{5.17}$$

where m is the rank of Θ. If $m < min(n,q)$ then both columns and rows in Θ are linearly dependent (the matrix is singular). Here the columnvectors of U, $u_1 \dots u_m$, are the orthonormal eigenvectors of $(\Theta\Theta^T)$, and the columnvectors of V, $v_1 \dots v_m$, are the eigenvectors of $(\Theta^T\Theta)$. σ_i are the singular values; σ_1^2 is the largest eigenvalue of $(\Theta\Theta^T)$ (or $(\Theta^T\Theta)$), σ_2^2 the second largest and so on. σ_m^2 is the smallest non-zero eigenvalue. The pseudoinvers of Θ is

$$\Theta^\dagger = V\Sigma^{-1}U^T \tag{5.18}$$

Here Σ^{-1} is diag $(\sigma_1^{-1}, \sigma_2^{-1} \dots \sigma_m^{-1})$. The smallest singular value, σ_m becomes the largest in the pseudoinverse. Consequently, the sensitivity of the pseudo-inverse to small errors (eg., noise) in Θ may be large if σ_m is small, that is, if the condition number

$$\gamma(\Theta) = \frac{\sigma_1}{\sigma_m} \tag{5.19}$$

is large. The key idea of the PCR estimator is to reduce this sensitivity by choosing only $k \leq m$ terms in the sum in Eq.(5.17).

5.3.2 Principal Component Regression.

Write the SVD in Eq. (5.17) on the alternative form

$$\Theta = t_1 p_1^T + t_2 p_2^T + \dots + t_m p_m^T \tag{5.20}$$

Here $t_i = u_i\sigma_i$ is the score vector (or latent variable) and $p_i = v_i$ is the loading vector for principal component i. Keep only the k first terms which may be distinguished from measurement noise, and let the matrices $P^{q\times k}$ and $T^{n\times k}$ include only these k most important directions. Then $\Theta \approx \Theta_k = TP^T$. The latent variables for a given temperature vector, θ, are then given by $t^{k\times 1} = P^T\theta^{q\times 1}$. The least square solution to $Y = TK_t^T$ becomes $K_t = Y^TT[T^TT]^{-1}$. The condition number of T, $\gamma(T) = \sigma_1(T)/\sigma_k(T)$, may be adjusted by selecting the number k. Since $P^{-1} = P^T$ (P is orthonormal), the overall estimator gain matrix then becomes

$$K_{PCR} = Y^T(\Theta_k)^\dagger = Y^TT[T^TT]^{-1}P^T \tag{5.21}$$

5.3.3 Partial Least Square (PLS) Regression.

This is a variation of the PCR method which recently has become popular among analytical chemists. The latent variables are here determined in order to have the greatest

covariance with the y-variables. It is an iterative process, which roughly (see Höskuldsson, 1988) may be described as follows:
For Θ find:

1. the largest eigenvalue a_1 and corresponding eigenvector w_1 of $\Theta^TYY^T\Theta$. Scale w_1 to length one.
2. the scores $t_1 = \Theta w_1$
3. the loadings $p_1 = \frac{\Theta^T t_1}{t_1^T t_1}$
4. the residual matrix $E_1 = \Theta - t_1 p_1^T$

For Y find:

1. the largest eigenvalue a_1 and corresponding eigenvector c_1 of $Y^T\Theta\Theta^TY$. Scale c_1 to length one.
2. the scores $u_1 = Yc_1$
3. the loadings $q_1 = \frac{Y^T u_1}{u_1^T u_1}$
4. the connection b_1 between the scores of θ and y: $b_1 = \frac{u_1^T t_1}{t_1^T t_1}$
5. the residual matrix $F_1 = Y - b_1 t_1 c_1^T$

Then start from the top with the residual matrices E_1 and F_1 in stead of Θ and Y, and continue until the matrix $E_k^TF_kF_k^TE_k$ has only small eigenvalues left. For a more exact description of the algorithm and its different versions, see Martens and Næs, 1989.

The estimator based on k factors is

$$K_{PLS} = Q(P^TW)^{-1}W^T \tag{5.22}$$

where the matrices $Q^{p\times k}$, $P^{q\times k}$ and $W^{q\times k}$ are formed by the vectors q, p and w introduced above.

The main advantage of the PLS-algorithm compared to PCR, is that it selects the directions in Θ which have the largest covariance with y, and thus ensures that these directions are treated first.

5.3.4 Scaling of variables (weight functions).

The objective of scaling is to improve the estimate by giving each temperature a weight corresponding to the inherent prediction ability.

The most common weight is the inverse of the standard deviation. This ensures that variable scaling (or variable transformations) do not bias the results. The weight for the i'th temperature is

$$W_{1i} = \frac{1}{s_{ci}} \tag{5.23}$$

We use s_{ci} as the standard deviation of the calibration set for temperature i, that is, it is the square root of the i'th diagonal element of $\frac{1}{n}(\Theta^T\Theta)$.

This weight simply scales all temperatures such that their changes are of the same magnitude. Since the change in terms of unscaled temperatures is small towards the end of the column, this means that measurements close to the ends will have a large weight, W_1. However, we know that this may not be a good approach because the noise is large (in relative terms) close to the ends. In order to take noise into account in the weighting, Martens and Næs (1989) suggest using the weight

$$W_{2i} = \frac{1}{s_{ci} + s_{e_k i}} \tag{5.24}$$

Here $s_{e_k i}$ is an estimate of the noise level, defined as the square root of the residual variance after k factors, i.e, the square root of the i'th diagonal element of $\frac{1}{n}(E_k^T E_k)$. This variance includes all contributions of model/data mismatch, i.e both noise and mismatch due to nonlinearities etc. Note that $s_{ci} = s_{e_0 i} \geq s_{e_k i}$, Finally, we propose to use the weight function

$$W_{3i} = \frac{1}{s_{ci}} \frac{s_{ci} - s_{e_k i}}{s_{ci}} \tag{5.25}$$

This weight is equal to W_1 when there is no noise, but gives zero weight to measurements where all variation is unexplained (due to noise).

To calculate the weights, we first performed the calibration once without weights. In the weight functions $k = 3$ was used for the binary mixture, and $k = 4$ in the multicomponent mixture. Typical examples of weight functions are given in Figure 5.8. We see that weight W_3 puts less weight on the column ends than W_1 and W_2.

5.3.5 Estimators for the example column.

The different PLS and PCR estimators are identified with an code sequence given in Table 5.3. A 'M' denotes a multicomponent mixture. A 'P' denotes that different pressure

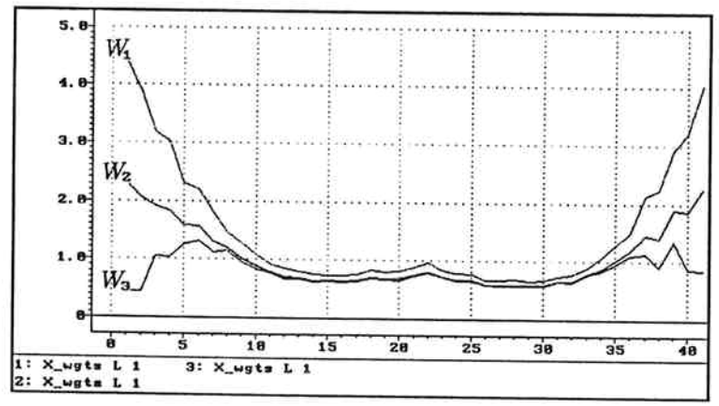

Figure 5.8: Weight functions W_1, W_2 and W_3 for Case n_2. (Untransformed data with 0.2 °C random noise.)

M	Multicomponet mixture.
P	Pressure variations of ± 0.1 atm.
L_Y	Log. transf. comp. only
L_T	Log. transf. comp. and temp. (ref.: boiling temp.)
L_θ	Log. transf. comp. and temp. (ref.: tray temp.)
n_0	no noise
n_1	0.1 °C noise
n_2	0.2 °C noise
W_n	Weight function n

Table 5.3: Estimator cases

levels of ± 0.1 atm are included randomly in the calibration set. L_Y denotes an estimator with logarithmic compositions and untransformed temperatures, L_T denotes logarithmic compositions and logarithmic temperatures, L_θ denotes the same, but with tray 1 and 41 (binary mixture), or tray 4 and 37 (multicomponent mixture) as reference temperatures, rather than the pure component boiling temperatures. Trays 4 and 37 are selected because they have minimum variance in the calibration set and are just outside the non-key separation area, see fig 5.5. The logarithm of the absolute value is used for temperatures 1–3 and 38–41. n_0, n_1 and n_2 denotes estimators with zero, 0.1 °C, and 0.2 °C normal distributed noise added to the calibration set. These are added to each measurements except for cases P where we add noise on the temperature differences $\theta - \theta_L$ and $\theta_H - \theta$. Note that estimators based on L_θ have a varying reference temperature, which will be corrupted by noise, whereas L_T and PL_θ do not. Finally, W_1, W_2, and W_3 denote the different temperature weight functions in section 5.3.4.

5.4 Results.

The static Explained Prediction Variance (EPV) (see section 5.2.6) for a number of cases are summarized in Table 5.4 and we shall study these results in more detail below. All estimators use PLS-regression unless otherwise stated.

5.4.1 Dynamic and static estimation

We shall first discuss the use of PLS-estimator n_0 (no noise) for the binary column. This uses no transformations on y and θ and no weighting. For the linear case (if we use a linear column model at the operating point) with three factors these estimates are identical to those obtained with the PCR-estimator studied by Mejdell and Skogestad (1990). They found this static estimator to perform excellently also when used dynamically and for feedback control. Typical simulation results for the linear case are shown in the left part of Figure 5.9. However, the column is strongly nonlinear and in this paper we also include nonlinearity. The corresponding simulations in the right part of Figure 5.9 show that the dynamic results are quite similar also in this case. From the figure the main problem seems to be the static prediction capability of the estimator, and we shall therefore use mainly static arguments to evaluate the estimators in the following.

No noise:	No. of factors						
	1	2	3	4	5	6	7
n_0	19.61	81.97	94.17	97.18	98.18	99.43	99.96
n_0L_Y	21.78	80.14	92.86	93.45	96.92	97.20	98.80
n_0L_T	19.72	96.38	**99.97**	99.98	99.99	100.00	100.00
n_0L_θ	32.90	95.39	**99.95**	99.96	99.97	100.00	100.00
n_0P	-2.31	46.77	75.71	92.19	95.50	95.95	97.59
$n_0L_\theta P$	19.16	94.90	**99.94**	99.97	99.97	100.00	100.00
Mn_0	10.66	48.02	56.78	88.35	89.58	91.50	91.94
Mn_0W_2	11.14	48.44	57.40	87.76	90.61	91.84	92.25
Mn_0L_Y	18.52	48.88	52.59	83.66	84.10	87.84	87.43
Mn_0L_θ	22.73	77.52	94.10	95.81	96.27	97.61	97.55
$Mn_0L_\theta W_2$	20.69	73.75	93.81	**95.87**	96.75	97.68	97.66
0.1°C noise							
	1	2	3	4	5	6	7
n_1	19.59	81.78	93.81	97.00	97.59	97.86	98.05
$n_1L_TW_3$	23.10	91.42	**98.89**	98.92	98.92	98.82	98.80
$n_1L_\theta W_3$	23.18	84.60	91.09	94.01	96.16	96.69	97.06
$n_1L_\theta W_3P$	26.89	91.05	98.25	98.78	99.04	99.08	99.04
0.2°C noise							
	1	2	3	4	5	6	7
n_2	18.87	81.10	93.78	94.92	94.49	94.42	94.47
n_2W_1	17.06	86.04	95.75	94.66	94.39	94.18	93.64
n_2W_2	20.40	84.65	95.66	95.36	94.74	94.70	94.12
n_2W_3	19.78	83.34	95.08	95.59	95.40	95.25	95.04
$n_2L_YW_3$	18.14	80.14	91.53	92.57	91.73	91.29	90.53
n_2L_T	12.50	78.41	81.90	84.04	87.59	90.63	91.16
$n_2L_TW_1$	22.65	86.65	95.44	96.25	96.70	97.22	97.33
$n_2L_TW_2$	22.78	87.66	96.43	96.99	97.30	97.64	97.59
$n_2L_TW_3$	23.04	89.07	**97.49**	97.68	97.86	98.14	98.05
$n_2L_\theta W_3$	26.41	84.53	86.59	87.43	90.07	89.10	88.52
$n_2L_\theta W_3P$	20.58	86.30	**98.01**	98.09	97.89	97.84	97.80

Table 5.4: EPV for different PLS estimators.

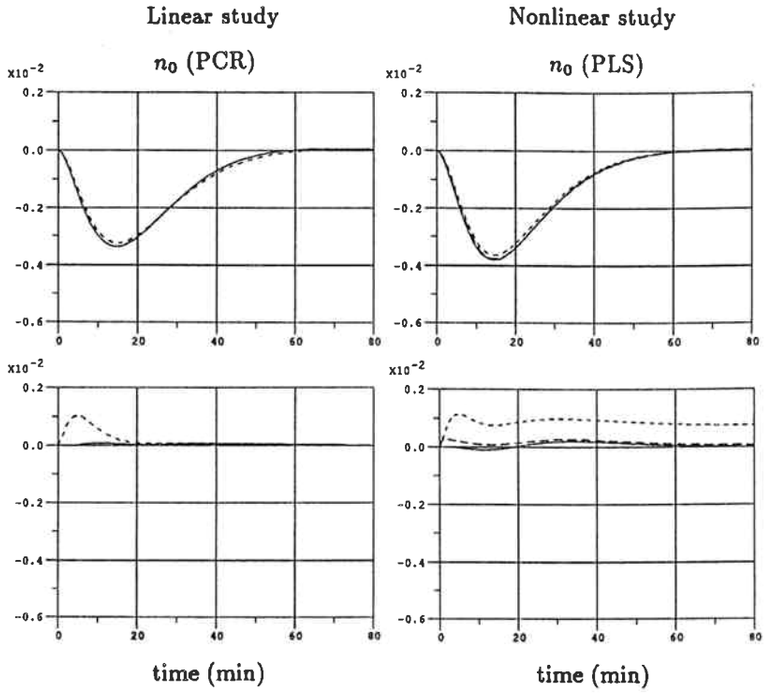

Figure 5.9: Closed loop responses of y_D for steps in feedrate (upper) and feed compositions (lower). Input to controller; Solid line: Perfect measurement, dotted line: Estimator with 3 factors, long dotted line: Estimator with 7 factors.

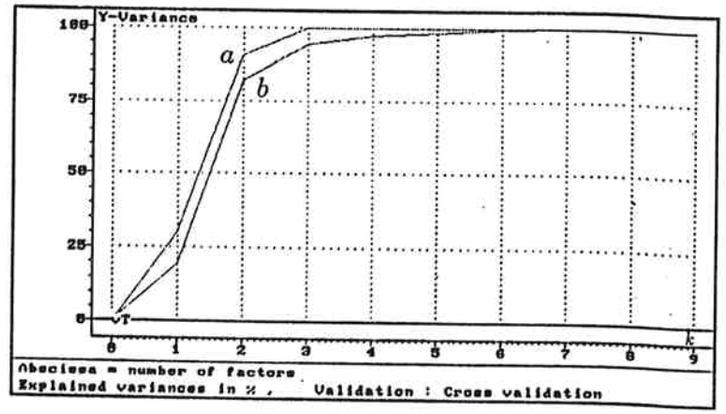

Figure 5.10: Effect of number of factors on Explained Y-variance, EPV (%), for case n_0 with no noise. a) Linear model, b) nonlinear model.

5.4.2 Effect of nonlinearity.

From the simulations in the right part of Figure 5.9 we see that increasing the number of factors in the PLS-estimator from three to seven almost removes the effect of nonlinearity. The same conclusion is obtained by considering the static EPV-values. In Figure 5.10 the EPV is plotted as a function of the number of factors. Since the column itself has only three degrees of freedom, three factors would account for 100% of the variance if the column were linear (small perturbations). However, because of nonlinearity, the actual EPV with three factors is only 94%, and the EPV increases by adding factors.

5.4.3 Influence of measurement noise.

However, the simulations above and the EPV-values are for the ideal case with no noise, and in practice the results with many factors will not be as good. Figure 5.11 compares EPV for different levels of measurement noise on the temperatures in the calibration set. The noise will corrupt the smallest factors, and after 3-5 factors there is no improvement of adding factors, and it may even reduce the prediction ability. We therefore see that in the presence of noisy measurements, it is doubtful to use additional factors to capture nonlinearity.

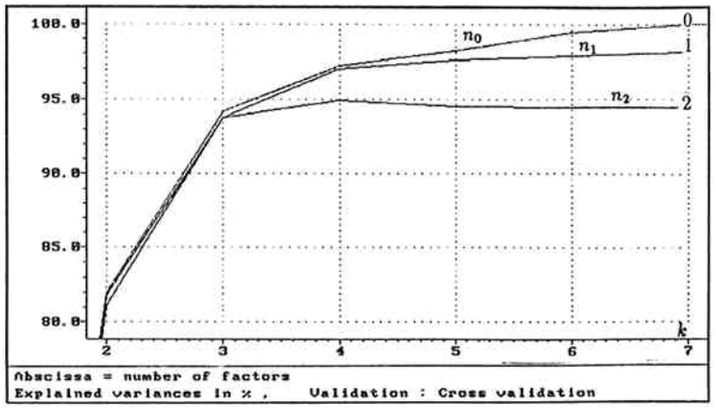

Figure 5.11: Effect of measurement noise on EPV for estimator n_i. $i = 0$: no noise, 1: 0.1 °C, 2: 0.2 °C.

5.4.4 Insights about directions in the temperature space.

Fig. 5.12 displays a typical plot of the three largest loading vectors, that is, how the different measurements are summed up to make the factors (latent variables). The first factor is due to the changes in external streams, D and B, and reflects moving the temperature profile up and down the column. The second factor is connected to changes in the internal streams, L and V, when D and B are held constant. It reflects the magnitude of separation in the column. The third factor is due to changes in feed composition.

5.4.5 Effect of pressure.

Figure 5.13 shows the EPV for the calibration set with total column pressure variations of 10%. From Figure 5.14 we see that the first factor, which has no predictive ability, mainly represents the pressure variation. The pressure variation may alternatively be taken care of by using differential temperatures.

5.4.6 Use of logarithmic transformations.

The results in Table 5.4 seem to indicate that use of logarithmic transformed compositions, i.e. $Y_D = ln(1 - y_D)$ and $X_B = lnx_B$, combined with *un*transformed temperatures (L_Y-

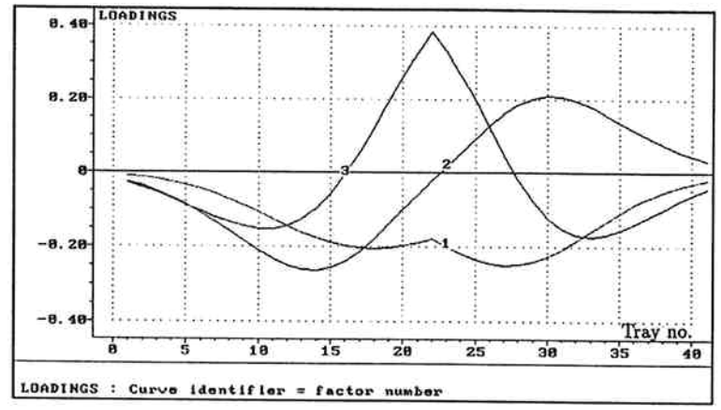

Figure 5.12: Loading plot (vector p_i) of first three factors for estimator n_0. Curve identifier: i, factor number.

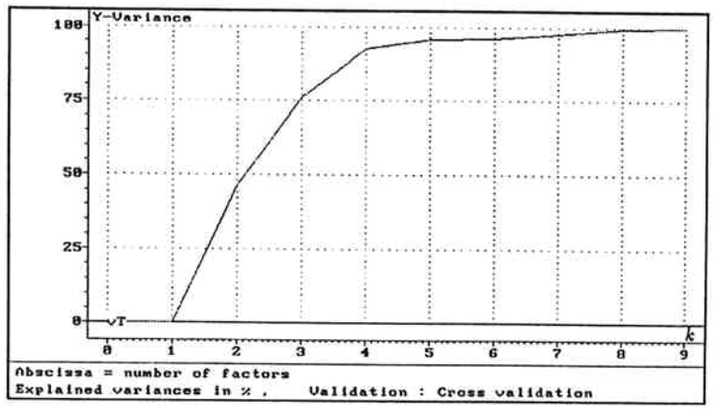

Figure 5.13: EPV for case n_0P with pressure variation.

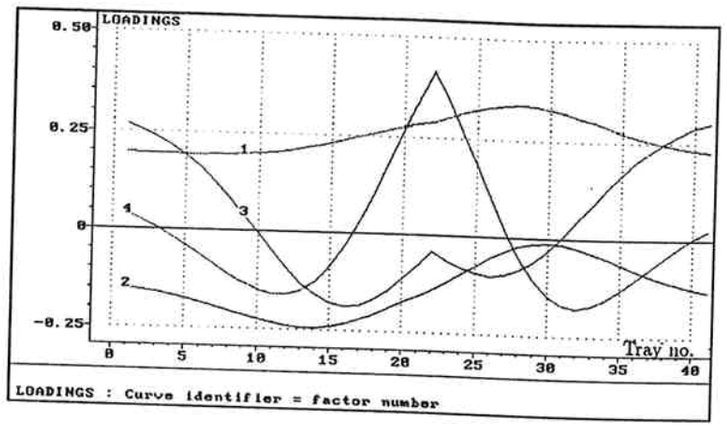

Figure 5.14: Loading plot for case n_0P with pressure variation. Curve identifier: Factor number.

estimators), generally has a negative effect on the estimate. However, the results are not quite comparable because the EPV is based on Y_D and X_B in stead of y_D and x_B. Other tests show that they are approximately equally good. But since the calibration minimizes the variance of Y_D and X_B in stead of y_d and x_b they have slightly different properties: The accuracy of the logarithmic estimator will be best in the pure region, and will never give estimates outside the region $0-1$. For feedback control it may be an advantage to use Y_D and X_B because this makes the controller tunings less dependent on operating conditions (eg., Skogestad and Morari, 1988b).

However, estimator performance is significantly improved by using logarithmic transformations also on the temperatures. We see from Table 5.4, that with no noise EPV is close to 100% after only 3 factors. This is the case also when pressure variations are included, that is, these are automatically taken care of when transformed temperatures L_θ are used.

5.4.7 Effect of weights on temperatures.

We shall consider the case with logarithmic temperatures. In cases n_0L_T and n_0L_θ with no noise there is no improvement of weighting the measurements, because the logarithmic transform will automatically weigh the temperatures similar to weight W_1. But when

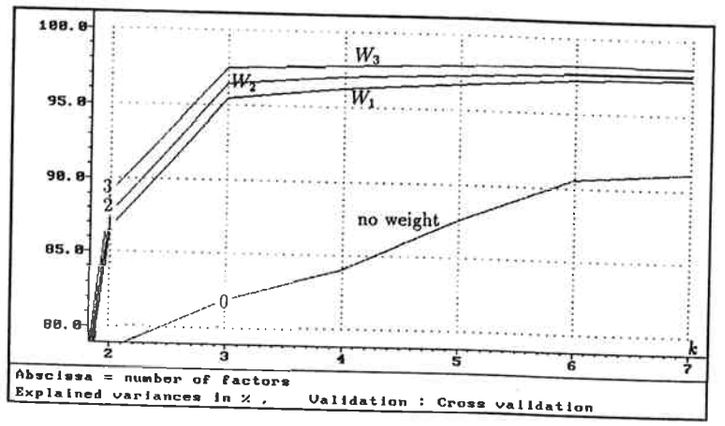

Figure 5.15: Effect of weights on EPV for estimator $n_2L_TW_i$ with logarithmic temperatures and 0.2 °C noise. Curve identifier: weight function i, 0: no weight.

noise is added to the calibration set, weighting is very important. Figure 5.15 compares different weight functions with 0.2 °C noise. Weight W_3 yields the best result.

5.4.8 Noise of reference temperaures

Case $n_2L_\theta W_3$ in Table 5.4 show that estimators using corrupted (noisy) reference temperatures perform poorly. The values of L_θ close to the location of the reference will then be very sensitive to noise. However, in practice temperatures close to each other are perhaps more likely to have correlated than independent noise. The results with the noise put on the temperature difference instead, such as $L_\theta P$ and L_T, may therefore be more realistic. Anyhow, the results demonstrate that logarithmic transforms may be quite sensitive to noise.

5.4.9 Multicomponent mixture.

The results in Table 5.4 for case Mn_0L_θ show that with no noise we obtain EPV-values in the range 94.1%-97.6% for static PLS estimators using logarithmic temperatures and 3-6 factors. We see that we need more factors compared to the binary mixture, mainly due to the additional degrees of freedom caused by the two additional components. However, we see that even with more factors, we do not attain the same prediction capability as for

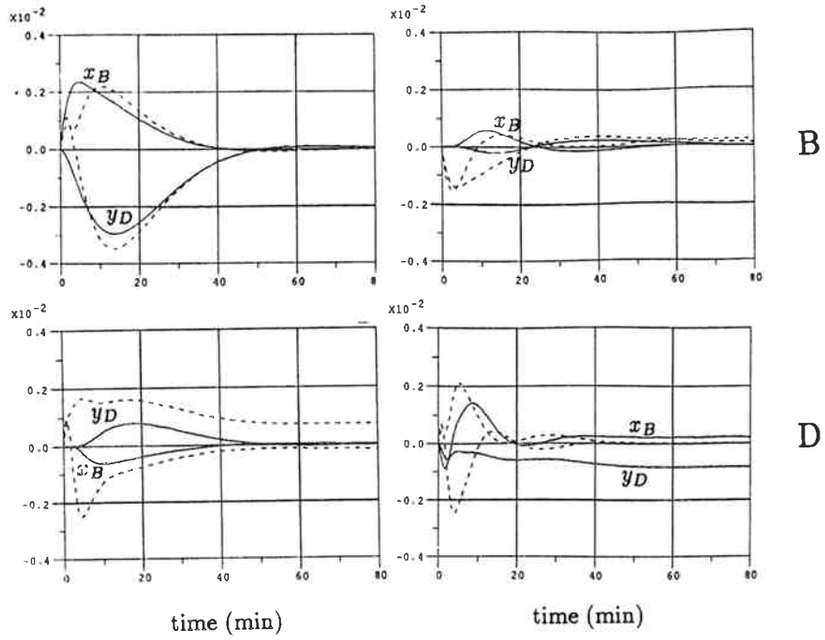

Figure 5.16: Closed loop responses of y_D and x_B for multicomponent case. Estimator $Mn_0L_\theta W_2$ with 4 factors. Results are shown for 20 % step in a) feedrate, b) feed composition z'_f, c) heavy non-key composition, d) heavy non-key composition when input to the controller is the estimate, $\hat{y}$. (In cases a–c y is used for feedback). Solid lines: y, dotted lines: $\hat{y}$.

the binary mixture. The improvement from using logarithmic temperatures is however substantial also in this case.

The simulations in Figure 5.16 illustrate the dynamic performance of the static PLS-estimator. The performance is somewhat worse than for the binary mixtures shown in Fig 5.9. The worst disturbance seems to be changes in heavy component. However case d in Fig. 5.16 demonstrates that the estimate works reasonably well for feedback control even here.

	Factors k						
Case	1	2	3	4	5	6	7
n_0	-9.64	0.90	0.06	0.14	0.01	0.49	0.00
n_1	-9.76	0.87	0.07	0.06	0.60	0.68	1.16
n_2	-9.63	0.91	0.05	0.03	-0.32	-0.23	-0.35
n_0L_Y	-9.26	1.00	0.01	0.35	4.60	0.86	0.01
n_0P	1.48	-1.70	4.99	0.02	0.13	0.34	0.59
$n_2L_TW_1$	-11.70	1.37	4.31	2.29	2.14	2.11	2.34
Mn_0L_θ	-5.96	1.64	16.54	4.11	-0.27	1.36	0.33

Table 5.5: Improvement in %-EPV using PLS rather than PCR estimator

5.4.10 Comparison of PLS and PCR.

In Table 5.5 the two methods are compared. The values of practical interest are those for 3–5 factors. In most cases the difference is small, although PLS is generally somewhat better.

5.5 Discussion.

Comparison with one temperature estimator. All results above were based on using all 41 temperatures for estimation. To compare with the conventional one-temperature control, we used the same calibration data to compute the EPV for an estimator using only one temperature. Different measure locations were considered for the case with binary mixture and 0.2 °C noise. To estimate y_D tray no. 9 was found to be optimal with $EPV = 88.7\%$ and for logarithmic compositions $EPV = 85.4\%$. This compares to $EPV = 97.5\%$ obtained with logarithmic estimator $n_2L_TW_3$ with three factors and using all temperatures. The relatively high EPV-values for the case with one temperature may explain why one temperature control is popular for composition control. However, the accuracy of the estimate is quite sensitive to the location, and EPV is reduced 4–5 % only two trays off tray 9. In addition to yielding better estimates, the use of multiple temperatures is therefore less sensitive to measurement location and to noise.

Neglected effects. The results have demonstrated that it is possible to obtain quite precise estimates with the PLS and PCR regression methods. However, these results are based on a simulation study where we neglected variations in tray efficiency, liquid

fraction in feed, reflux subcooling, local pressure drops, etc. Variations in these will affect the temperature profile to some extent. However, we believe that most of these variations will be too small to be distinguished from noise, or will not significantly change the relationship between θ and y.

Noise level. Our mixture has a relative volatility of 1.5, corresponding to a temperatures difference between the two key components of only 13 °C. Nevertheless, for the binary mixture we were able to obtain prediction capability (EPV) of 97.5% with only three factors for the case with 0.2 °C noise. This noise level is about 1.5 % of the temperature difference. Hence, a mixture with a temperature difference of 40 °C should be able to cope about equally well with a noise level of about 0.6 °C .

Coping with nonlinearity and noise. A major problem for the estimator is that the temperatures at the column ends, which are most representative for the product streams (at least in the binary case), also are most affected by nonlinearity and noise.

We have proposed three different methods to deal with this problem:

- Using more factors
- Weighting according to temperature variation and noise
- Logarithmic transforms

Using a larger number of factors than the number of degrees of freedom is helpful when the noise level is not too high. The reason why this may help is that the product compositions have different nonlinear relations to different temperatures. These differences will appear as extra directions (factors) in the linear temperature space. However some of these differences are small and may be distinguished from noise. A useful rule is to increase the number of factors until they no longer have any significant positive effect on the EPV. For distillation columns, the typical optimal number of factors are 3–5.

Weighting of variables is commonly used for dealing with different kind of measurements. This is to prevent that the measurements with the largest nominal changes dominate. In our distillation column only temperature measurements are used, so one might think that weighting is unnecessary. Nevertheless, weighting proved useful. The reason is that the temperature changes are very small at the column ends (in the calibration set their standard deviation is only 6% of the temperature with the largest variation), but even in the presence of noise they do contain useful information about the end compositions. By using weights we avoid that the PLS method discards the use of these temperatures.

However, the noise should also be taken into account, and weight functions W_2 and even more W_3, which include information about the noise, yield better results.

Compared to PCR, there is also a kind of weighting inherent in the PLS-method (Höskuldsson 1988), since it searches for directions in the $\Theta^T Y Y^T \Theta$, in stead of only $\Theta^T \Theta$. The weighting with the matrix YY^T gives temperatures which have the largest covariance with y larger weight when making the factors. The comparison between PLS and PCR shows that these "weightings" improved the estimates in some cases, although the difference was quite small.

The use of logarithmic transformations of temperatures was clearly the single method with the greatest effect. It appears to be a very powerful method to cope with the nonlinearity in distillation columns, and also automatically gives the temperature measurement at the ends a greater weight. However, when the temperatures are corrupted with noise, the noise will also be transformed, and have a relatively large effect on these end temperatures. Therefore, as seen from Figure 5.15, it is absolutely necessary to weight the transformed data to take this into account. As already mentioned, one should also take action to avoid very small or negative temperature differences before transforming the temperatures.

Choice of reference temperature. For multicomponent mixtures the reference temperatures should be located some distance away from the ends: 1) They should be in the section where the concentration of the off key component is almost constant (See Fig: 5.5). Much of the off-key component's contribution to the temperature will then be cancelled. 2) They should be located as far out to the ends as possible to capture the nonlinearity. A method which coincides with this two criteria is to use the temperature with least variation in the calibration set.

Measurement selection. The results above are based on using all 41 temperatures as measurements. This is of course not necessary. However, the number of measurement should at least be equal to the number of factors needed for prediction. For example, to capture 3 factors, we need at least 3-5 temperatures. The highest number applies to estimators which use differential temperatures, for example, L_θ. Additional temperatures will mainly reduce the effect of measurement noise. As a simple method to select the location of temperature measurements, we recommend identifying the peak elements in the K-matrix for the weighted (scaled) variables. The number of peaks is usually the same as the number of factors. As an illustration, consider Figure 5.17 which displays the elements in K for the weighted untransformed temperatures for y_D using PLS-estimators

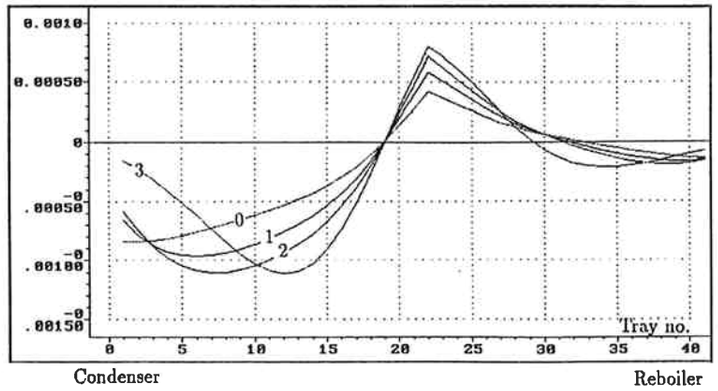

Figure 5.17: Estimator vector K (y_D) for PLS-estimator n_iW_2. Curve identifier i: 0 - no noise, 1 - 0.1 °C, 2 - 0.2 °C, 3 - ∞ °C (the same as no weighting.)

n_0W_2, n_1W_2 n_2W_2 and n_0 (the weight W_2 is different in the cases as it depends on the noise level). We see that when the noise is increased it is better to locate the temperatures further from the end.

A simple procedure for measurement selection and obtaining the estimator is: 1) Determine all possible measurement locations. 2) Determine expected magnitudes of outputs (y) and all variables (disturbances) affecting the system. 3) Perform simulations that include the expected variations (Use factorial design and make sure the entire output space is spanned). 4) Add random noise to all measurements. 5) Transform the variables, and perform the PLS-regression. 6) Determine the number of optimal factors, and weigh the variables with a suitable weight function, for example, W_3. 7) Do the PLS-regression once more with the weighted variables, but without noise on the measurements, and find from the weighted K-matrix where to place the measurements. 8) Perform the final calibration to obtain the estimator with the selected set of weighted measurements.

The advantage with this procedure, compared for instance to Moore(1986), is that for each measurements it takes explicitly care of both its correlation to the outputs and its noise level.

5.6 Conclusions.

The problem addressed in this paper belongs to a broad class of problems concerning how to handle multiple measurements in an estimator. Depending on the magnitude of correlation with the estimated variable and its sensitivity to noise, the different sensors should be weighted to give the best estimate. The paper has shown that this indeed also applies for sensors of the same type such as the temperatures in a distillation column.

For distillation columns the main difficulty of using linear estimators is the nonlinearity in the process. It is found that the logarithmic transforms of compositions and temperatures proposed in this paper is a highly powerful means of coping with this nonlinearity. Together with weight functions that place less weight on sensors with large noise, these transforms are found to give a substantial improvement in the prediction ability.

Use of logarithmic temperatures, L_θ, which makes use of differential temperatures, gives the additional benefit of counteracting pressure variations.

The results for multicomponent mixtures indicate that the estimator may perform well in a wide range of applications. Using section reference temperatures at locations with the least temperature variance, will make logarithmic transforms useful also here.

Besides being an efficient method of obtaining estimators, the standard multivariable calibration techniques yield added benefits, such as insight in the process, good statistical information about the prediction ability, and a method for sensor location.

NOMENCLATURE (also see Table 5.4)

B - Bottom product flow rate
D - Distillate flow rate
EPV - Explained Prediction Variance in %. See sec. 5.2.6
F - feed rate
k - number of factors used in estimator
K - estimator constant
L - reflux flow rate
L_T - logarithmic temperatures based on boiling points
L_θ - logarithmic temperatures based on reference temperatures
t - vector of latent variables
T - matrix of latent variables (t) for calibration runs

T^b - boiling temperature of pure component

V - boilup from reboiler

x_B - mole fraction of light component in bottom product

y_D - mole fraction of light component in distillate

y - output vector $(y_D x_B)^T$

Y - matrix of outputs (y) for calibration runs

z_F - mole fraction of light component in feed

W_1, W_2, W_3 - weight functions for temperature scaling

Greek symbols

$\alpha_{i,j}$ - relative volatility between components i and j

γ - condition number

σ_i - i'th singular value

θ - temperature vector

θ_L, θ_H - reference temperature in top and bottom of column

Θ - matrix of temperatures (θ) for calibration runs

Subscripts

H - heavy key component

L - light key component

Superscripts

' - pseudobinary basis

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Chapter 6

Experimental setup.

The experimental investigations were performed on a pilot plant distillation column at the Norwegian Institute of Technology, Department of Chemical Engineering. The objective was to check that the results obtained from theoretical simulation studies were useful in practice, and to gain further insight into the estimation problem by dealing with a real system. During the first part of the Dr. ing. study much time was spent on rebuilding the column, improving the instrumentation, and writing software for the control system to prepare for a later implementation and testing of the estimators.

6.1 Distillation pilot plant.

6.1.1 The distillation column.

The experimental distillation column (Figure 6.1) is about 5 meters high, has a diameter of 125 mm, and consists of eleven sieve-trays. The space between the trays is 300 mm. A tube with a diameter of 35 mm is a combined outlet weir and downcomer. (Figure 6.2) The downcomers are equipped with liquid seals and are located 42 mm above the tray below. The advantage of this arrangement compared to a system with inlet weirs, is that it gives more active hole area, though it might give some poorer liquid distribution. The entire column is made of 2 mm stainless steel and consists of flanged sections. It is insulated with rock wool. Inspection glasses are provided at the feed point and upper and lower tray levels.

The pilot plant is basically the same as the one used by Loe (1976), although various modifications have been performed. The rectifying section and the feed tray have been changed and are now identical to the stripping section by means of a downcomer system

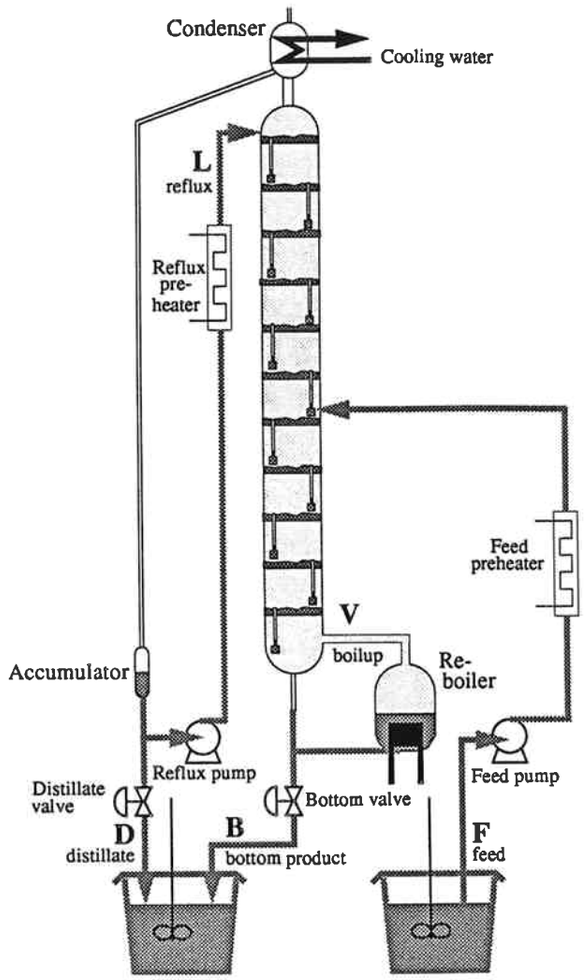

Figure 6.1: Pilot Plant Distillation Column

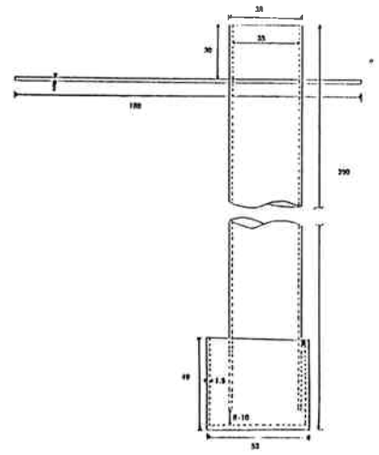

Figure 6.2: Downcomer arrangement.

and hole area. All outlet weir levels in the column have been changed to 30 mm. (Figure 6.3). Each tray now has 65 holes, and the diameter of the holes has been increased from 2.2 to 2.7 mm. The changes have been performed to better meet the recommendations in the literature (Ludwig, 1971; Huang and Hodson, 1958; Hunt et al., 1955 and Mayfield, 1952.) with respect to percentage hole area, vapor speed in empty tower, and pressure drops. The vapour and liquid rates may now be run from about 20 to 100% of the capacity without flooding, weeping, or noticeable entrainment.

The liquid houldup inside the column is approximately 3.5 litres during operation. The liquid transport delay from top to bottom of the column is approximately 15 seconds, and the liquid fraction over weir is about 0.1. This fraction is rather small compared to industrial columns (typically values there are 0.5). No K_2-effect (Rademaker et al., 1975) has been observed.

More details about the column are found in Wahl (1989).

6.1.2 Peripheral Equipment

The reboiler consists of a 15 litre kettle with 6 electrical heating elements, each of 2.5 kW power. In normal operation it contains about 6 litres of liquid.

A water-cooled total condenser is placed right on top of the column. A vent with an extra condenser ensures atmospheric pressure. The accumulator tank is reduced to 435

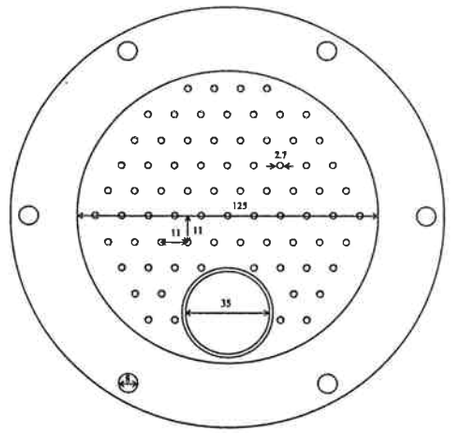

Figure 6.3: Sieve-tray, mounted between two flanged sections.

ml and placed at the floor.

The feed enters the column at tray five (counted from bottom). Both the feed and reflux flows are provided by two Wallace & Tiernan metering pumps with a capacity of one litre/min. The pumps have a constant motor drive (1425 rev/min.) and a variable stroke length driven by a servo motor. Changing the flows from zero to 100 % of their capacity takes approximately one minute. Two preheaters with power capacities of 2 and 5 kW are connected to the reflux and the feed pipe line respectively.

The distillate and bottom product streams are adjusted by two Foxboro needle style control valves. Their capacities are about 400 ml/min.

6.2 Instrumentation.

A cromel-alumel thermocouple is placed in the reboiler and in the liquid at the centre of each tray. (Figure 6.3). These 12 thermocouples are connected to a Data Translation terminal panel card which provides cold-junction compensation and a 200 times amplification of the signals. The computer's 12 bits A/D-card will then provide a bit resolution of the temperatures of approximately 0.05 °C.

There are also thermocouples placed in the feed and reflux lines. Each is used in connection with a analog PID-controller and a preheater to maintain desired constant

temperatures in the flows, usually the boiling point temperatures.

Three Foxborough Differential Pressure Cells measure the column pressure drop and the liquid levels of the accumulator and reboiler. (It is also possible to read these quantities manually.)

Two solenoid valves are used for sampling the bottom and top product. A 3-way valve is used for the distillate and is located right below the condenser, while a 2-way valve is used for the bottom product. It is located below the lower tray in the connection line between the column and the reboiler. The two control valves are equipped with actuators and voltage-to-current transmitters so they can accept control voltage signals from 0-10 Volts. The servo motor of the reflux pump and the reboiler power supply have corresponding equipment.

The product composition is analyzed by a Chrompack 9000 Gas Chromatograph with a flame ionization detector.

6.3 Data sampling and control system.

The data sampling and control unit consists of:

1. Hewlett Packard 9000, model 216 personal computer.
2. Multiprogrammer, model 6942A for I/O-cards.
3. Control panel for switching and adjusting control parameters.
4. Think Jet writer.
5. HP -plotter.

All units are interconnected by HPIB (IEEE 488) interfaces. The software is written by myself in HP-Basic and consists of approximately 1800 statesments.

6.3.1 Sampling.

The twelve temperatures and the three differential pressures are sampled every second. The 12 bits A/D-converter in the multiprogrammer is converting signals in the range ± 1 Volt. From the multiprogrammer the values are read in one batch into the computer where they are checked for outliers or faults. Every fifth second an average value of the

accepted values is stored into an array. The computer has 1.5 Mbyte memory, and is capable of storing runs for about 2.5 hours without writing the data to hard disc.

A digital output card handles the solenoid valves for liquid composition sampling. The sampling is done during one second.

6.3.2 Control.

Output signals to the four actuators are updated every fifth second. These are the two controller valves for the product flows, the input power to the reboiler, and the metering pump for the reflux. The range of all output signals is 0–10 Volts.

The four control loops are implemented as ordinary PID-controllers with anti-windup. The anti-windup is implemented such that the integral part of the controller stops when the actuators are either in maximum or minimum position. Different control configurations are stored in separate files such that they may be read into the computer whenever desirable. The control parameters to each configuration are initialized by stored values from a previous run.

All control parameter values, setpoints, and output signals (when the loops are in manual) may be changed at any instant from the computer by either writing in desired values, or adjusting the existing values from the control panel. The digital reading of the control panel is done every second.

All output signals and all changes of parameter setpoints and auto/manual switches of the control loops are also stored in arrays.

There exists an analog backup system for the control.

6.3.3 The data program.

The whole realtime program consists basically of interrupt sub-routines. Many interrupt commands are available in HP-Basic language and have facilitated the writing of the program, for instance variable priority setting of each sub-routine. The sub-routines are compiled to get a higher computer speed.

All instant values of inputs, outputs, product estimates, and control parameters are continuously displayed in real units on the screen. Two of these variables are selected at any time to be shown graphically. The time horizon of these plots is updated automatically. The change between graphic mode and display mode is almost instant.

The graphic commands are the same to the screen as they are to the plotter. An

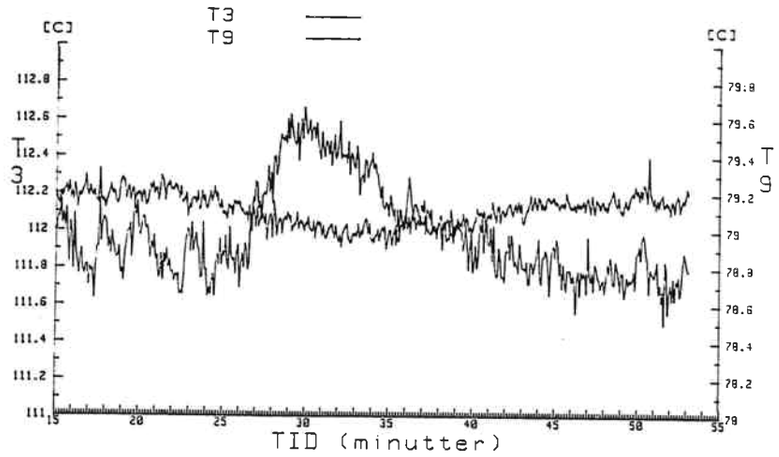

Figure 6.4: A typical plot on screen during operation.

example is given in Figure 6.4. After finishing an experimental run the setpoints and control parameters are available for plots too. One may also write selected parts of the data to the printer or to an ASCII-file.

One advantage with using Basic is that the variables declared in the program will not loose their values when the program is stopped. Using arrays is therefore a relatively safe and very quick means of data processing in realtime mode.

6.4 Binary component system.

In the search for a suitable binary system, the following criteria were considered:

1. The system should have a high relative volatility in order to get a high purity distillation column. (The column has only eleven trays.)

2. The system should perform quite typically, i.e. it should not be too un-ideal. This would also support the use of simple simulation programs.

3. The system should be relatively convenient to handle, i.e have low toxicity, relatively low flammability, boiling temperatures around 100 °C, and be easily analyzed.

4. The system should be inexpensive.

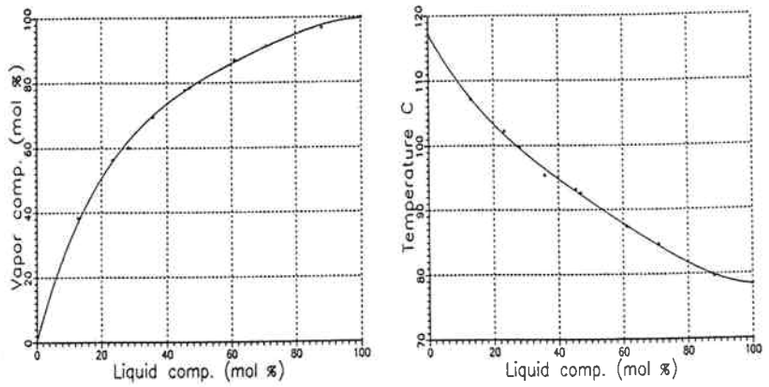

Figure 6.5: Equilibrium and temperature diagram.

The binary system ethanol/1-butanol was found to fulfill most of these requirements. The system is quite ideal and follows the Raoults law quite closely (Brunjes and Bogart, 1943). Figure 6.5 shows the equilibrium diagram and the corresponding boiling-point temperatures for the system (Hellwig and van Winkle, 1953).

The equilibrium data cited in most data books (e.g Chu et. al., 1956; Hirata and Nagahama, 1975; Gmehling and Onken, 1977) are that of Hellwig and van Winkle (1953), Gay (1927), and to some extent also Brunjes and Bogart (1943). While the first two references give almost constant relative volatility, the last one does not (Figure 6.6). However, since this seems to be much less cited, a constant relative volatility value of 4.3 is assumed and used in simulation programs.

The relation of density and heat of vaporization to the temperature is found in Gallant (1968) for both alcohols. Antoines Parameters used for temperature calculation in simulation programs are taken from Boublík et. al., (1973).

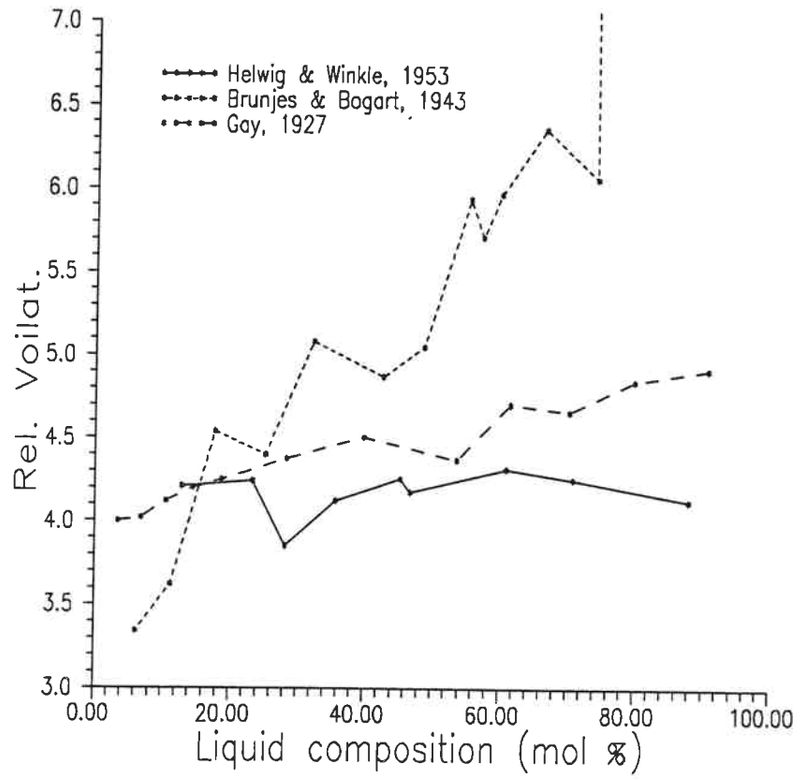

Figure 6.6: Relative volatility as a function of liquid composition.

Chapter 7

Product Composition Estimator in a Pilot Plant Distillation Column

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Abstract

Results are given for the implementation of a static Partial Least Square (PLS) regression estimator for product compositions on a high-purity pilot plant distillation column. Temperatures on all 11 trays are used as inputs to the estimator. Several estimators were tested off-line to compare their performance, and one estimator was used on-line for dual composition control. It was found that the estimators perform very well when appropriate logarithmic transforms and scalings are used. Since the estimator is static, the implementation is straightforward. An estimator based only on experimental data gave excellent performance over a wide range of operating points. Estimators based on simulations did not perform quite as well, and the bias had to be adjusted when changing from one operating point to another. Nevertheless, since it may be difficult to obtain good experimental data in an industrial setting, this estimator is probably most useful in practice. In the paper we discuss how to combine information from simulations (basic modeling) and experiments.

7.1 Introduction.

Product composition analyzers for distillation columns, such as gas chromatographs, have large investment and maintenance costs, in addition to unfavourable large measurements delays. The most popular means of product control is therefore temperature control (Kister, 1990), which provides an easy, fast and inexpensive means of composition control.

The temperature selected for control is usually located at a tray some distance away from the column ends, because the products may be extremely pure, and the temperatures variations are too small compared to the noise. Furthermore, pressure variations and off-key components will interfere the relationship between product composition and temperature and favors locating the measurements away from the ends (Rademaker et. al., 1975). However, at this location the temperature will be strongly influenced by the composition of the feed and of the product at the other column end.

An important issue in conventional temperature control is therefore to find the best measurement location by making proper compromises between these considerations.

However, some of the interferences may be handled by using more measurements. Since the column pressure has about the same effect on all temperatures in the column, the pressure variation may for instance be compensated using temperature differences. This requires an additional temperature measurement which preferably is located at a tray where the composition is almost constant.

Along the same line of thoughts are the proposals to use double differential temperatures. Yu and Luyben (1984) proposed to use the other differential temperature for off-key component compensation, while Luyben (1969) and Boyd (1975) proposed to use it for column pressure drop compensation. However, these ideas do not seem to be widely applied.

On the other hand, for the special case of high purity columns with large relative volatility between the components the use of multiple temperatures has found some applications because the conventional temperature control is difficult. In these columns the main temperature drop will take place in a small region consisting of only a few trays. Quite small deviations from normal operating point may lead to a control temperature outside this region. On the other hand, the location of this temperature front (region) will have large correlation to the compositions and may alternatively be the control object. Bozenhart (1988) located the front by scanning multiple temperatures for the maximum temperatures drop between two trays. Another simple way of tracking the temperature

front is to use an average of many tray temperatures (Luyben, 1971). Whitehead and Parnis (1987) used a weighted average of many differential temperatures in a C_2-splitter.

A more rigorous means of using multiple temperatures in to provide an estimator for product compositions. Many approaches have been proposed, e.g. by Brosilow and coworkers, (Weber and Brosilow, 1972; Joseph and Brosilow, 1978) who used temperatures together with stream measurements and a linearized process model, and by Marquard (1988), who used a state space observer for the location of the temperature front.

In another paper by the authors (Mejdell and Skogestad, 1990a) three different estimators were compared on a rigorous basis using *linear* data for a 40 trays high-purity binary example column with a constant relative volatility of 1.5. These estimators were the dynamic Kalman-Bucky filter (Kalman and Bucy, 1961), the static Brosilow Inferential Estimator (Weber and Brosilow, 1972; Joseph and Brosilow, 1978), and the static Principal Component Regression (PCR) Estimator. It was found that for feedback control the static PCR estimator performed almost as well as the Kalman filter. The reason is that the temperatures and compositions have similar dynamic responses. The Brosilow Estimator was very sensitive to model error for this ill-conditioned plant with large RGA-values (Skogestad et al., 1988). Mejdell and Sogestad (1990a) therefore recommended using the simple regression estimator, which is obtained simply by considering corresponding values of temperatures and composition.

Mejdell and Skogestad (1990b) further investigated the use of regression estimators in a *nonlinear* study. The impact of different levels of temperature noise, pressure variations and off-key components were also studied. The estimators were found to yield satisfactory estimates, especially when using proper weighting (scaling) and logarithmic transforms. The use of multiple temperatues by the estimators effectively counteracted the effect of pressure variations, measurement noise, off-key components and the nonlinearity in the column. The PLS and PCR estimators were also compared, and the first was found to be slightly better.

These results are the starting point of the present paper. We will present some of the results from an implementation of the PLS-regression estimator on a pilot plant distillation column, and discuss some issues that may be important when implementing the estimator on industrial columns. The pilot column separates a binary mixture of ethanol and butanol and has temperature measurements on all 11 trays.

7.2 The experimental equipment.

7.2.1 The pilot plant column.

The experimental distillation column (Figure 7.1) consists of eleven sieve-trays and has a diameter of 125 mm. The space between the trays is 300 mm. A kettle type reboiler is heated by electrical elements with a total power of 15 kW. The reboiler contains 6–7 litres of liquid. A water-cooled total condenser is placed right in top of the column and is open to atmosphere. A small accumulator tank is placed at the floor. It contains about 250 ml distillate.

The feed and reflux flows are provided by two metering pump with a capacity of one litre/min. The pumps have a variable stroke length driven of a servo motor. Both flows have preheaters with temperature controllers. The distillate and bottom product flows are adjusted by two needle style Foxboro control valves. The bottom product will normally have the same composition as the liquid from the bottom tray (insignificant thermosyphon effect in the reboiler).

Two solenoid valves are used for sampling the liquid from the bottom and top product. They are placed below the bottom tray, and after the accumulator. Because of the small accumulator size, this will imply a composition lag of only 1-2 minutes. The liquid samples are analyzed off-line by a Chrompack 9000 Gas Chromatograph.

Each tray in the column is equipped with a cromel-alumel thermocouple placed in the liquid. There is also a thermocouple in the reboiler. Differential pressure cells are used for measuring pressure drop in the tower and for liquid levels in the accumulator and reboiler.

The column may be run under a wide range of operating conditions. The vapor and liquid rates may be run from about 20 to 100% without flooding, weeping or serious entrainments.

7.2.2 Data sampling and control.

Sampling and control are provided by a Hewlett Packard 200 model 16 personal computer with a Multiprogrammer model 6942A for I/O-cards. The software is written in HP-Basic.

The twelve temperatures and the 3 differential pressures are sampled every second. Every fifth second an average value is stored, and control signals sent to the actuators. They are the two controller valves for the product flows, the power to the reboiler, and the metering pump for the reflux flow.

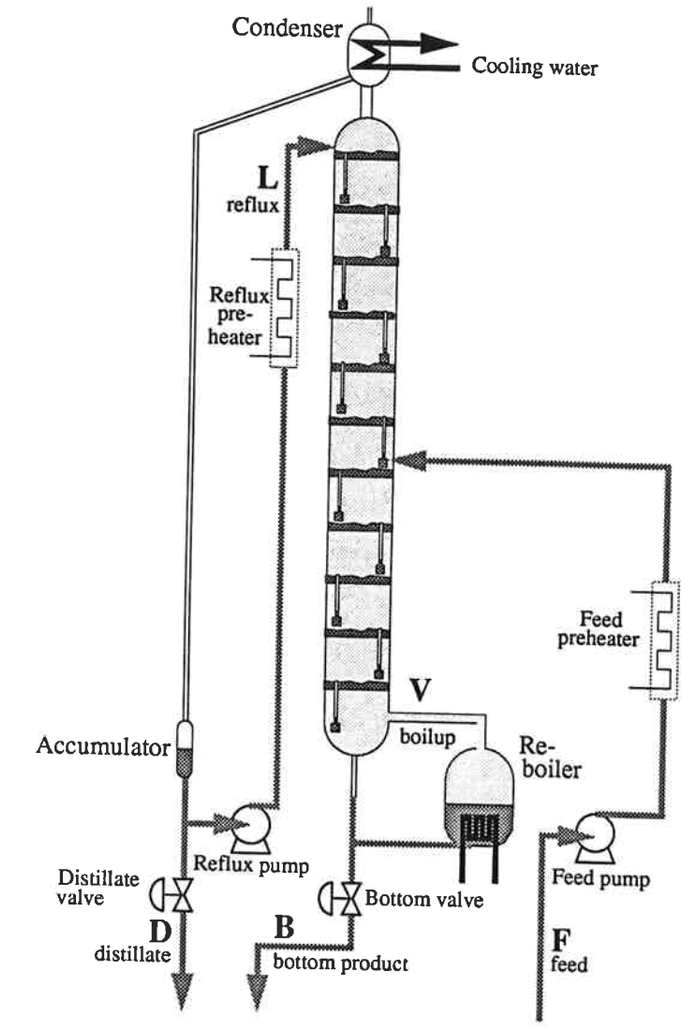

Figure 7.1: Pilot Plant Distillation Column

Liquid sampling of the distillate and the bottom products are controlled by the computer and taken precisely every 2^{nd} minute.

The controller loops are implemented as ordinary PID-controllers with anti-windup.

7.2.3 Chemical Components.

In the search for a suitable binary mixture, we considered the following criteria:

1. The mixture should have a high relative volatility in order to get a high purity distillation column. (The column has only eleven trays.)
2. The mixture should be reasonably ideal to avoid unusual behavior to bias the results.
3. The system should be relatively convenient to handle, i.e. have low toxicity, relative low flammability, boiling temperatures around 100 °C, and be easily analyzed.
4. The system should be inexpensive.

We found the mixture ethanol/1-butanol to suit most of these requirements. It has nearly constant relative volatility of 4.3 (Hellwig and van Winkle, 1953).

7.3 Data treatment and multivariate regression.

Multivariate calibration (regression) is a statistical approach to obtain a linear estimator using a "training" set of known values of inputs and outputs to the estimator.

For the distillation column we want to obtain the matrix K in

$$y = K\theta + k_0 \tag{7.1}$$

Here y denotes the outputs of the estimator (top product, y_D, and bottom product, x_B) and the θ, the inputs (temperatures). The vector k_0 is the bias or mean of the outputs.

A training set (calibration set) of n runs of corresponding values of θ and y are obtained and lined up in two matrices Y and Θ such that measurements of each run are placed in one row. Deviation variables are used, that is, all measurements are first centred around the mean in the calibration set, y_0 and θ_0. The data are in most cases also weighted (scaled). Using 2 y-variables and 12 θ-variables we get

$$Y^{n\times 2} = \Theta^{n\times 12} K^T \tag{7.2}$$

where K has the dimension 2×12. We search for the solution

$$K^T = \Theta^{\dagger} Y. \tag{7.3}$$

where $\Theta^{\dagger}$ denotes a pseudo-inverse of Θ.

Different calibration methods will yield different solutions. Using Singular Value Decomposition (SVD) we obtain the Principal Component Regression (PCR) estimator. To avoid collinearity and an ill-conditioned estimator we delete the directions in Θ with small singular values (corresponding to noise). The number of remaining non-zero singular values, or equivalently the number of principal components (factors) used, will give the rank, k, of the pseudo-inverse $\Theta^{\dagger}$. In our application on distillation columns k is typically 3–5 (Mejdell and Skogestad, 1990b)

The Partial Least Square (PLS) regression method used in this paper is very similar, but it also takes into account the covariance with the y-variables when doing the decomposition. This may yield an estimator with fewer factors than PCR (Höskuldsson, 1988). However, Mejdell and Skogestad (1990b) found that the differences were rather small for their distillation column example. The procedure is given by Martens and Næs (1988), and is also explained by Mejdell and Skogestad (1990b).

7.3.1 Use of transformed variables.

The composition and temperature profiles are nonlinear functions of the operating variables. Logarithmic transformation of the product compositions, i.e.

$$Y_D = \ln(1 - y_D); \quad X_B = \ln x_B \tag{7.4}$$

has been proposed by several authors (e.g., Joseph et al., 1976) as an effective way to linearize the *response* (with L, V, F, z_F etc. as independent variables).

The column composition profile may also be linearized using logarithmic transformations, for instance

$$X = ln(\frac{x}{1-x}) \tag{7.5}$$

for binary systems. Skogestad and Morari (1988) showed that this transformation also linearizes the dynamic response. Temperature is often a nearly linear function of composition. Mejdell and Skogestad (1990b) therefore proposed to use the following transformation to linearize the temperature response and profile

$$L_T = \ln(\frac{\theta - T_L^b}{T_H^b - \theta}) \tag{7.6}$$

Here T_L^b and T_H^b are the boiling temperatures of pure light and heavy components, respectively. Column with pinch zones around the feed will not have a linear profile.

Instead of using boiling temperatures, one may use the transformation

$$L_\theta = \ln(\frac{\theta - \theta_L}{\theta_H - \theta}) \tag{7.7}$$

where θ_L and θ_H is some *reference temperature* in the top and the bottom of the column, respectively. For binary mixtures, one may use the temperature at the column end, which is very close to the boiling temperature, and which does not change very much with operating condition. To avoid large effect of noise on the temperatures closest to the reference temperatures one should also specify a lower permitted limit on the difference temperatures in equations (7.6) and (7.7).

Using reference temperatures also provides pressure compensation of the temperature measurement.

7.3.2 Scaling of variables, weight functions

In all cases the data were centred around the mean. In most cases the temperatures were weighted. Weight 1 is given by

$$W_{1i} = \frac{1}{s_{ci}} \tag{7.8}$$

This is the inverse of the standard deviation of temperature i in the calibration set and ensures that, for example, variable scaling does not bias the results. Weight 3 (the numbering follows Mejdell and Skogestad, 1990b) is given by

$$W_{3i} = \frac{1}{s_{ci}} \frac{s_{ci} - s_{ei}}{s_{ci}} \tag{7.9}$$

Here s_{ei} is the residual standard deviation between the model predictions and the observations. s_{ei} takes into account both noise and mismatch due to nonlinearity. In our example s_{ei} is the residual after three PLS factors based on a preliminary calibration without weighting. Weight W_3 is equal to W_1 when the model is perfect (no noise), but gives zero weight to measurements when all the variation is unexplained ($s_{ci} = s_{ei}$).

7.4 Experiments and simulations.

7.4.1 Experimental Steady State Runs.

In order to obtain a calibration set, 19 different steady-state runs were performed on the experimental column. The runs were first checked for consistency and outliers. Two

No.	$F(mol/min)$	$z_F(\%)$	$y_D(\%)$	$x_B(\%)$
1	4.12	45.02	99.20	0.37
2	4.14	45.71	99.64	0.64
3	3.65	34.63	99.67	0.88
4	3.64	34.32	96.82	0.16
5	4.57	34.58	98.81	0.16
6	4.57	34.53	99.15	0.27
7	3.65	34.53	99.50	0.95
8	3.63	54.61	96.81	1.10
9	4.56	54.61	95.54	0.11
10	4.55	54.36	99.10	2.66
11	3.64	55.28	99.13	0.22
12	4.58	55.60	99.27	2.18
13	4.22	50.79	99.01	0.36
14	4.48	50.70	97.71	0.22
15	3.36	44.03	99.50	0.31
16	3.35	42.95	99.14	0.25
17	3.39	45.70	99.41	0.33

Table 7.1: The 17 experimental runs used for calibration.

runs were deleted from the calibration set during this check. The remaining 17 runs used for calibration are listed in Table 7.1. To ensure that the different directions should be present in the calibration set, a fractional design was adapted. The obtained values of y_D and x_B show some minor deviations from the original design. Nevertheless, the runs do have a good spread. We stress that it may be very difficult and time-consuming to obtain such good data on an industrial column.

The column profile was stabilized by controlling the temperatures on tray 3 with the reboiler heat input, and tray 9 with the reflux pump. When the column temperatures had been constant values for at least 10 minutes, samples of the feed and the product streams were taken. In addition, the average and the standard deviation of all temperatures, pressures and output signals during the last 5-10 minutes were calculated and stored.

7.4.2 PLS-estimators based on experimental runs.

Different transforms of the experimental data give three different PLS estimators, denoted E1, E2 and E3.

- *Estimator E1* uses the 12 temperatures and the product compositions without doing any logarithmic transformations. The temperatures were weighted with the weight

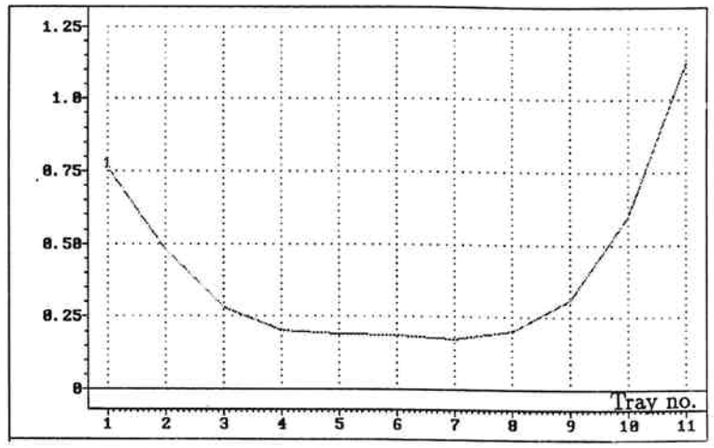

Figure 7.2: Weight W_1 for estimator E1

function W_1. The weight is shown in Figure 7.2.The optimal number of factors was found to be four.

- *Estimator E2* contains also four factors, but was obtained using the logarithmic transforms Y_D and X_B in Eq. (7.4) . The data were centred, but no weighting was performed.

- *Estimator E3* uses in addition to the logarithmic transform of the compositions, also the transform L_θ (Eq. 7.7) on the temperatures. The temperature in the reboiler, θ_0 was not found suitable as reference temperature, so the temperature in tray 1 was used in stead. The number of inputs to the estimator then became nine for this estimator (compared to 12 for E1 and E2). The data were centred and weighted with the weight function W_3. The optimal number of factors was found to be three. W_3 and s_e is plotted in Figure 7.3

7.4.3 PLS-estimators based on simulation runs.

For simulating the experimental column a steady-state simulation program assuming constant relative volatility and constant molal flows was employed. From experimental runs

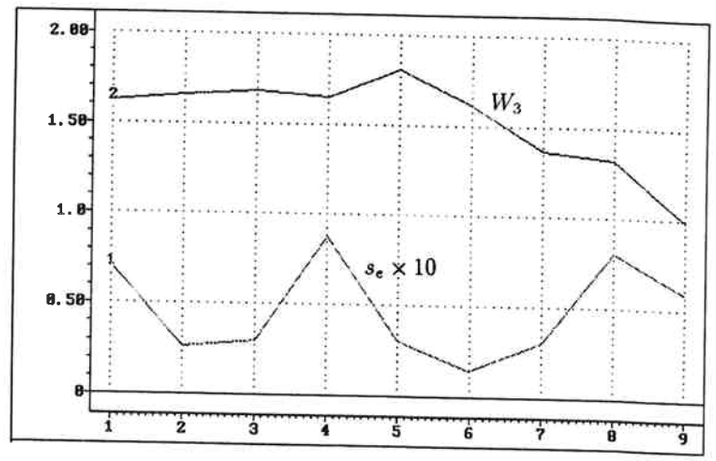

Figure 7.3: Mismatch $s_e \times 10$, and corresponding weight W_3 used for estimator E3. Logarithmic transformed temperatures are used.

a correlation between the column pressure drop ΔP (atm) and the boilup V (mol/min) was found and included in the simulation program:

$$\Delta P = 0.0166 - 0.0014021V + 0.000343822V^2 \tag{7.10}$$

From literature data (Helwig and van Winkle, 1953; Gay, 1927) the relative volatility of ethanol/butanol was estimated to be 4.3. To obtain a model of the column one generally adjusts the number of theoretical trays to match the experimental data. We used a constant Murphee tray efficiency η_M throughout the column. To obtain the estimators we used 32 different simulations runs as listed in table 7.2. Simulations were performed (and estimators obtained) for the following two cases

1. Estimator S1: Using an average Murphees tray efficiency, η_M of 0.82.

2. Estimator S2: Using a correlation between the Murphee efficiency and the boilup V and reflux L (mol/min):

$$\eta_M = 0.040898L - 0.0464262V + 0.928233 \tag{7.11}$$

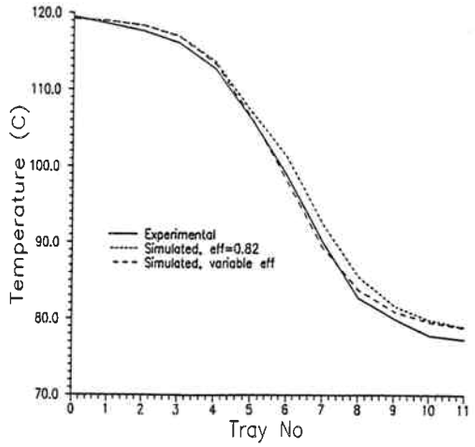

Figure 7.4: Comparison of temperature profiles for Run 16

During the experiments L and V varied in the range 3–15 mol/min. These two calibration sets gave rise to estimators S1 and S2 respectively. A typical temperature profile comparison is shown in Figure 7.4. The match with the experimental data is somewhat better for case 2.

Both estimators included the same logarithmic transforms and weight function as E3. The s_{ei} in weight function in equation (7.9) were found by first corrupting the data with 0.1 °C random noise and performing a preliminary calibration. Afterwards the weight function from this calibration was used with the original uncorrupted data in a new calibration step to yield S1 and S2.

7.4.4 Dynamic Test runs.

Two test runs with large composition variations were performed for comparing the different estimators. At distinct times, usually every second minute, a liquid sample was taken and analyzed off-line. Various feed and composition disturbances and setpoint changes were introduced during these tests. The column was controlled using the LV-configuration, i.e. the top composition was controlled by the reflux and the bottom composition by the boil-up.

F	z_F	y_D	x_B	P	F	z_F	y_D	x_B	P
4.5	0.5000	0.9900	0.0100	0.993	5.0	0.4000	0.9700	0.0300	0.993
4.2	0.4875	0.9962	0.0189	1.000	4.0	0.4000	0.9700	0.00333	0.991
4.6	0.5375	0.9913	0.0262	1.003	4.0	0.4000	0.99667	0.0300	0.990
4.0	0.4750	0.9956	0.0087	0.991	5.0	0.4000	0.99667	0.00333	0.998
4.3	0.4250	0.9738	0.0151	0.990	4.0	0.6000	0.9700	0.0300	1.010
4.8	0.5625	0.9934	0.0115	0.996	5.0	0.6000	0.9700	0.00333	0.997
4.7	0.5250	0.9700	0.0132	1.005	5.0	0.6000	0.99667	0.0300	0.990
4.5	0.4625	0.9772	0.0300	0.998	4.0	0.6000	0.99667	0.00333	0.999
4.1	0.4125	0.9801	0.0058	0.997	4.25	0.4500	0.98268	0.01732	0.996
5.0	0.4375	0.9950	0.0038	1.004	4.75	0.4500	0.98268	0.00577	1.005
4.4	0.6000	0.9849	0.0044	0.995	4.75	0.4500	0.99423	0.01732	0.993
4.3	0.4500	0.9924	0.0173	0.992	4.25	0.4500	0.99423	0.00577	0.992
4.9	0.5125	0.9942	0.0066	0.992	4.75	0.5500	0.98268	0.01732	1.005
4.6	0.5750	0.9868	0.0228	1.007	4.25	0.5500	0.98268	0.00577	0.993
4.8	0.5500	0.9827	0.0076	0.999	4.25	0.5500	0.99423	0.01732	1.002
4.2	0.5875	0.9885	0.0050	1.010	4.75	0.5500	0.99423	0.00577	0.990

Table 7.2: Specifications of F (mol/min), z_F, y_D, x_B and P (atm) to obtain simulated temperature profiles. Feed is saturated liquid.

In the first test run, denoted DYN1, the column was operated by temperature control of tray 3 and 9. The column was switched between one-point control and two-point control. In one-point control larges changes in reboiler power were made, while in two-point control large setpoints changes were performed. The column was also subjected to disturbances in feed rate, F, and feed composition, z_F, of about 30 %.

In the second test run, DYN2, the estimator S2 was used in the feedback loop, and setpoint changes in the estimated values of y_D and x_B were performed. In addition 25 % increase in feed rate were introduced at time t=29, 10% decrease in feed rate at t=43 min, and 30% decrease in feed composition at time t=53 min. The LV-configuration was used, that is, reflux L is used to control top composition, and boilup V for bottom composition. The estimator S2 was corrected for bias before start.

Controller tunings for test run DYN2.

Each composition control loop was first submitted to a Ziegler-Nichols tuning test, letting the other loop stay in manual. These individual the Ziegler-Nichols PI-parameteres were then detuned by a factor f to compensate for interactions between the loops.

$$k = \frac{k^{ZN}}{f}; \quad \tau_I = f\tau_I^{ZN} \tag{7.12}$$

Data taken during 10 min for Run 3				
Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	119.1208	0.0145
Temp. tray 1	(°C)	:	117.6565	0.0312
Temp. tray 2	(°C)	:	115.7841	0.0498
Temp. tray 3	(°C)	:	112.2051	0.1026
Temp. tray 4	(°C)	:	107.0069	0.1371
Temp. tray 5	(°C)	:	99.4882	0.1676
Temp. tray 6	(°C)	:	92.5084	0.1531
Temp. tray 7	(°C)	:	85.3724	0.0987
Temp. tray 8	(°C)	:	80.5095	0.0516
Temp. tray 9	(°C)	:	79.0260	0.0295
Temp. tray 10	(°C)	:	77.6493	0.0203
Temp. tray 11	(°C)	:	77.5407	0.0123
Reboiler Level	(Cm)	:	7.9115	0.0551
Accumulator Level	(Cm)	:	12.8806	0.1015
Diff. pressure	(Cm H_2O)	:	16.6909	0.0476
Output signals to actuators:				
Reboiler duty	(Volt)	:	3.0499	0.0000
Distillate pump	(Volt)	:	2.4296	0.0337
Bottom valve	(Volt)	:	8.7820	0.1436
Distillate valve	(Volt)	:	5.0953	0.0994

Table 7.3: Data from a typical experimental run.

This is similar to the BLT procedure of Luyben (1986).

Based on the results of Skogestad and Lundström (1990) who studied PID-control of a similar column we first selected $f = 2$. However, additional detuning was found necessary and $f = 2.5$ was used.

7.5 Results.

7.5.1 Experimental steady state runs.

The results of all runs are given in appendix A. In Table 7.3 the results from a typical run are shown. The standard deviations of the temperatures in the middle of the column are approximately 10 times larger than at the ends. They are evidently related to the slope of the temperature profile, as seen from the dotted line in Figure 7.5. Consequently, the

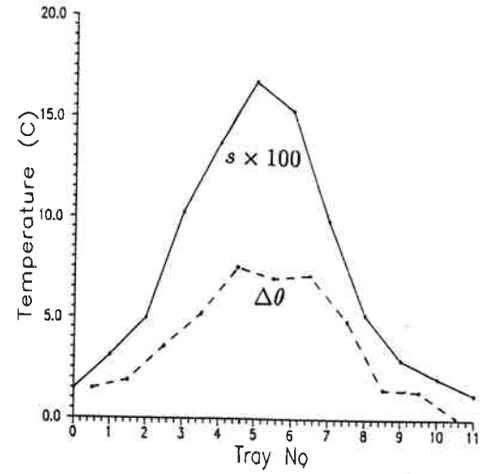

Figure 7.5: Comparison of standard deviation of the temperature measurements and the temperature difference $\Delta\theta$ between the trays. Steady state experiment Run 3.

main noise factor for the temperatures seems to be connected to liquid flow on the trays and not to the measurement device.

In Fig. 7.6a the temperature profiles for runs 5, 6, 7 and 8 are displayed. The corresponding logarithmic profiles are seen in fig 7.6b. The linearizing effect on the profile is clear, except for the top section of run 8 which has a pinch zone around the feed tray.

7.5.2 Experimental test DYN1.

The estimator were compared off-line using experimental temperature data from DYN1. The estimates of the experimentally based estimators E1 and E2 are displayed in Figure 7.7. The estimator E1 performs well for y_D, but not as well for x_B. Although it tracks the main changes, it has a tendency to overdo them, and gives also negative values of x_B. On the other hand, the bottom product estimates are excellent for E2, while the top product estimates show some steady state offsets. Note that the use of logarithmic transformed compositions in this case guarantees that the estimates of x_B and y_D stay between zero and one.

The effect of using logarithmic transforms both for compositions and temperatures is

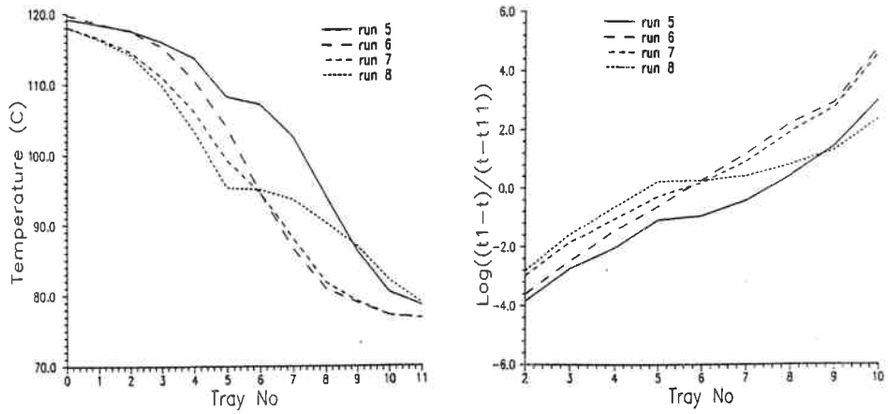

Figure 7.6: Temperature profiles for runs 5–8. a) Temperatures b) Logarithmic transformed temperatures.

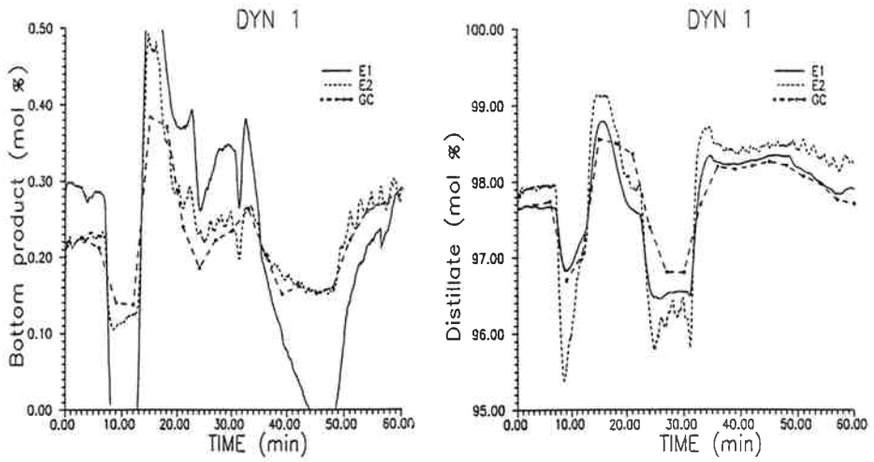

Figure 7.7: Performance of estimators E1 and E2 in test DYN1.

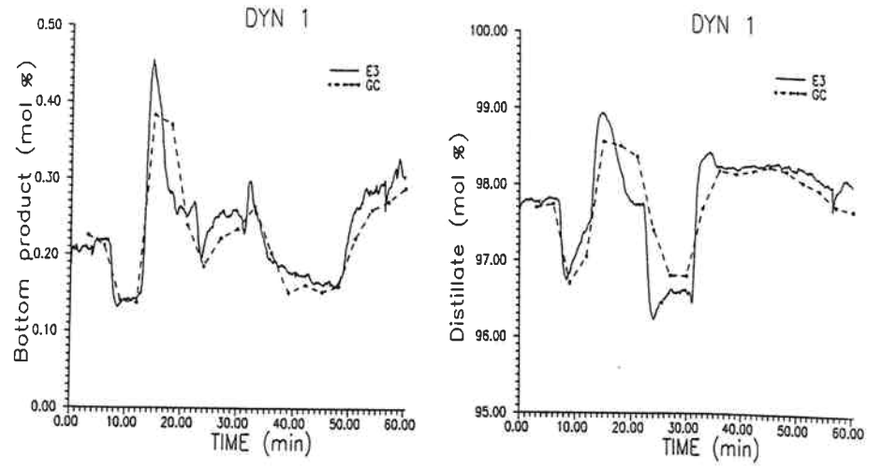

Figure 7.8: Performance of estimator E3 in test DYN1

shown in figures 7.8 where estimator E3 is employed. The estimates are excellent both for top and bottom compositions. Note that the bias term k_0 was not adjusted from its original value for any of the experimental estimators, E1, E2 and E3.

The performance of the estimators based on simulations, S1 and S2, are shown in Figure 7.9 The difference between S1 and S2 is minimal. In both cases the bias term k_0 in the estimator had to be adjusted for off sets before start. Although the estimators based on simulations are not as good as the experimental estimator, E3, they still show reasonably good performance.

7.5.3 Experimental test DYN2

In Figure 7.10 the setpoints and the *estimated* outputs are shown for the dynamic test DYN2, where estimator S2 was used on-line as part of the control loop. The controller tracks the setpoints very well, and the interaction between the loops does not seem to cause problems. In Figure 7.11 the *analyzed* compositions are compared with the estimate. We see that the S2-estimates deviate substantially for the bottom composition when moving to the new operating point.

For comparison the estimates of the experimental obtained estimator E3 is also dis-

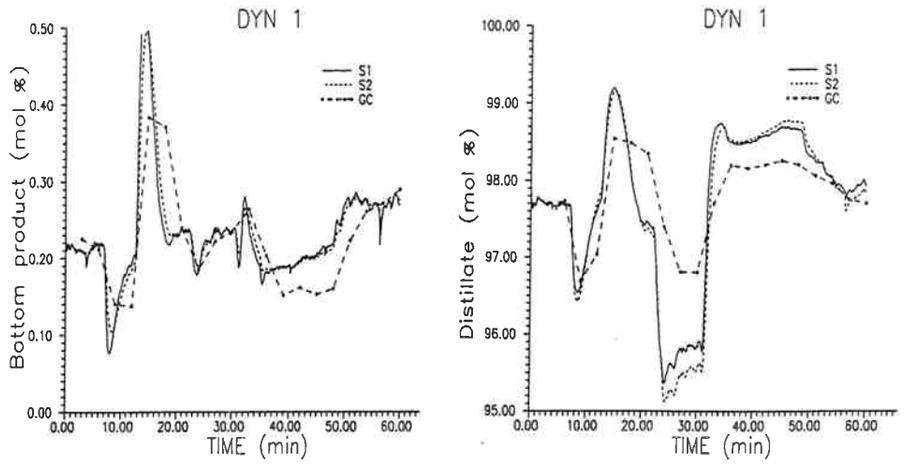

Figure 7.9: Estimators based on simulated data with *constant* (S1), and *variable* (S2) tray efficiency in test DYN1

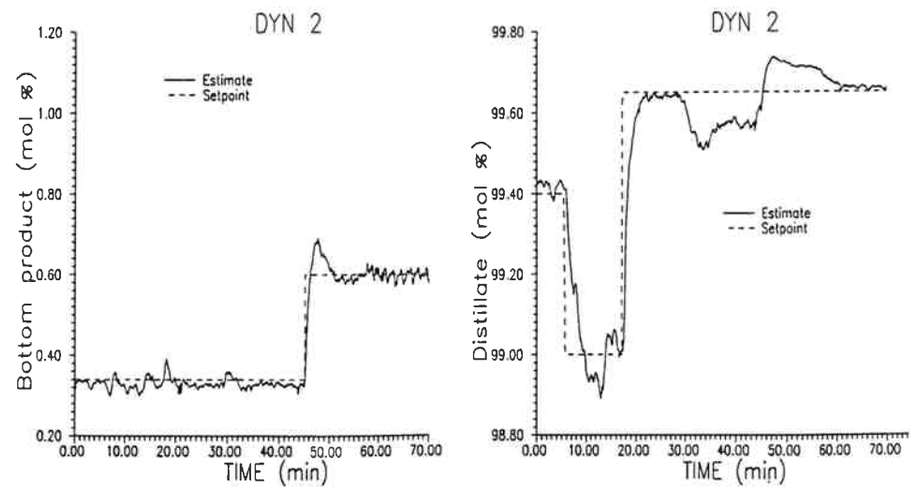

Figure 7.10: Control performance of estimated compositions when using estimator S2 in closed loop. (Test DYN2)

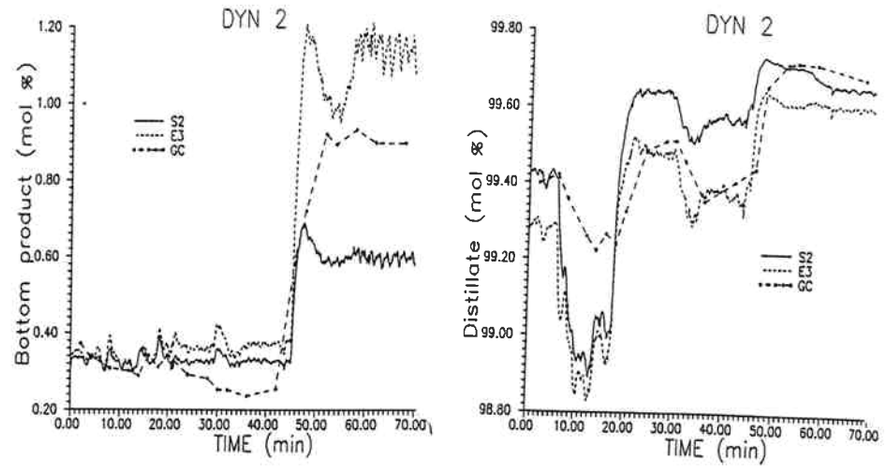

Figure 7.11: Performance of estimators S2 and E3 in test DYN2.

played in Figure 7.11. We note that E3 is much more sensitive to changes in the bottom product. Again, it was not subjected to any off-set adjustments, whereas the bias for S2 was adjusted.

The trend of the other estimators E1, E2 and S1 was similar as for the test DYN1.

7.6 Discussion.

The results confirm that a static estimator is sufficient for the distillation column. The estimates are generally a little ahead in time compared to the actual compositions. This is mainly due to the lag in the accumulator and the transport delay from tray one to the solenoid valve for bottom product sampling. This elimination of the lag is clearly an additional advantage of using temperture measurements for feedback control.

The accuracy of the estimators is also satisfactory, especially for the experimentally based estimators. Even without adjusting the bias these estimators gave very little steady-state offsets. The experimental calibration runs were obtained over an extended period of time (more than a month) and about half a year before the dynamic test DYN2. This indicates that it may not be necessary to update these estimators.

Experimental Estimators.

A comparison between the experimentally obtained calibration estimators, E1 and E2 for test DYN1, shows that E1 performed best for the top composition and E2 best for the bottom composition. The reason is the difference in purety for x_B and y_D in DYN1: x_B varied from 0.15 to 0.40 mole %, while $1-y_D$ varied from 1 to 3 mole %. The logarithmic transforms of the compositions (E2) will perform best in the pure range, that is, for x_B.

The estimator with best overall performance is E3, which seems to provide accurate estimates over a wide range of operations. This is primarily due to the linearizing effect of using logarithmic transformed temperatures. This confirms the results of Mejdell and Skogestad (1990b) who introduced logarithmic transformed temperatures and found them to give a substantial improvement in the steady state accuracy.

Controller Tuning.

The tuning of the control loops with estimator on line was straight forward. The Ziegler-Nichols tuning procedure proved to work although a substantial detuning was necessary. The estimator (and thereby also the controller) employs temperatures from both sections. One should consequently expect additional interactions between the loops. In this column, however, the interactions was not a large problem. In case it should happen to be a problem, one might include additional punishment into the weight function of the temperatures located far away from the estimated product.

Simulation Estimators.

A comparison of the two simulation based estimators, S1 and S2, shows small differences. The effect of varying tray efficiency in the simulation runs thus seems to be of minor importance for this column.

The static accuracy of the simulation estimator S2 was not satisfactory for the bottom product in the test DYN2. This estimator must consequently be updated when changing from one operating point to another. The experimental obtained estimator E3 performed better. It may therefore give insight to look at the differences of the K-matrix elements between estimator E3 and S2 as shown in Figure 7.12a. It is mainly the feedtray element (tray 5) that differs. Changing this element in estimator S2 from -0.6 to -0.1 gives an excellent response for DYN2 as shown in Figure 7.13a. Alternatively, one may shift the K-values for S2 one tray as seen in Figure 7.12b. This gives the response in Fig. 7.13b, which is very similar to E3. This illustrates that the estimator may be quite sensitive for for mismatch between the simulated and the experimental data for tray numbers where the K-matrix elements are subjected to large changes from one tray to another.

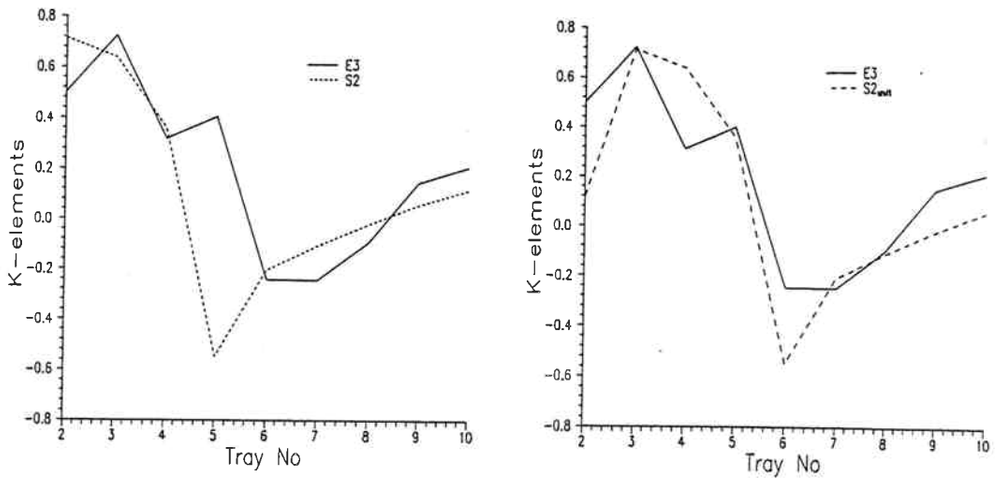

Figure 7.12: Elements in Matrix K for x_B

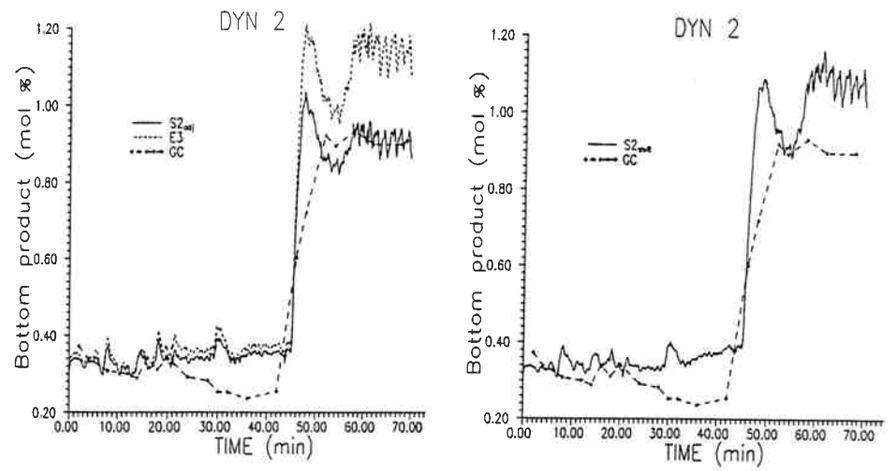

Figure 7.13: Performance of estimator S2 with a) adjusted K-element for tray 5, b) shift in tray numbers.

For a given estimator, one might use some test runs, such as test DYN1 and DYN2, to "adjust" a coefficient in the k-matrix as discussed above. A more rigorous approach would be to get a better estimator in the first place. For our column we could possibly have improved the simulation based estimator by including

1. Different tray efficiencies η_M in different sections.
2. Variable noise in stead of constant noise when performing weight W_3 for S2, e.g. according to Figure 7.5
3. Constant feed temperature rather than boiling point temperatures.

For our experimental column the first proposal would probably have minor importance since the difference in performance between S1 and S2 are very small. A more realistic noise would have given the feed tray temperature less weight, and a weight function W_3 which is more similar to the one used by S3. The last proposal would probably had the largest affect on the estimator. In the experimental column the feed temperature controller was set to a fixt value (boiling temperature of $z_F = 0.5$). This will not give a constant liquid fraction in the feed, as was assumed in the simulation runs. The last two items explain probably some of the difference in the k-element for the feedtray.

The reason why we care about the simulated based estimator is of cause that experimental calibration runs may be difficult to perform on many industrial columns in operation, and one has to rely on simulations. In particular, it is difficult to ensure that all the "directions" in the space of independent variables (y_D, x_B, disturbances) are sufficientlty exited.

The problem is then to adapt the simulated estimator to the real column. Although the above proposals may help, there will always be some mismatch between simulated and experimental runs left. There are consequently a need for more systematic methods.

Experimental data give a good representation of the true system, but it may be difficult to obtain reliable data which span the desired range of operation. On the other hand, simulations may not represent the true system as accurately, but it is easy to use the model to generate changes which are difficult to do experimentally. Also, there may be effects or disturbances on the real system which are not represented by the simulation model. This discussion leads to the conclusion that the optimal estimator should combine both simulated and experimental data. In some sense, this is done since the simulation model is obtained by adjusting the tray efficiency to match the experimental data. However,

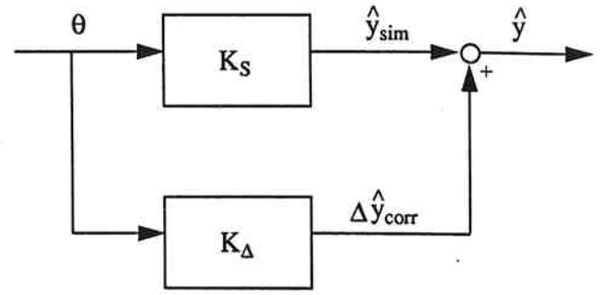

Figure 7.14: Block diagram for a combined estimator based on simulations ($\hat{y}_{sim}$) and corrected (Δy) using experimental data.

the results in this paper show that this is not sufficient, that is, the experimental data contains additional information.

One possible approach is shown in Figure 7.14.

$$\hat{y} = \hat{y}_{sim} + \Delta\hat{y}_{corr} \tag{7.13}$$

The simulation based estimator K_S is obtained first. This gives rise to the estimate $\hat{y}_{sim}$. The correction $\Delta\hat{y}_{corr}$ is found from the available experimental runs. The data matrices for the correction estimator corresponding to equation (7.2) become

$$\Delta Y = Y - Y_{sim} = \Theta_{exp} K_\Delta^T \tag{7.14}$$

The basic idea is to use the simulation based estimator, K_S, to capture effects ("directions") due to different feed compositions and product composition which may be difficult to excite in the real column. This estimate is then corrected by the experimental "correction estimator", K_Δ. In directions which are not exited by in the experiment the correction is only a constant term (bias), as for estimators S1 and S2. On the other hand, in directions where the experimental data has adequate excitations it should use the entire temperature profile. One important issue will be to ensure that the noise and uncertainty

in the experimental obtained data runs do not corrupt the estimate, by for example using a conservative number of factors in the correcting estimator. This approach may include an up-dating procedure for the correction estimator to handle long terms changes in the distillation column.

7.7 Conclusions.

The paper addresses the implementation of a Partial Least Square estimator on an pilot scale distillation column. An experimentally based estimator, with logaritmically transformed temperatures and compositions, gave excellent performance over a wide range of operating points. The need for up-dating of this estimator was minimal.

Estimators based on only simulated data showed reasonable performance. However, when changing to different operating points the steady-state bias had to be corrected. An important area of future work is to find estimators which efficiently combine data based on simulations and experiments.

NOMENCLATURE

B - Bottom product flow rate

D - Distillate flow rate

F - Feed rate

e_{ei} - Residual standard deviation of temperature on tray i.

E_k - Residual data matrix of the temperatures after extracting k factors.

$E1 - E3$ - Estimator based on *experimental* calibration runs.

K, k_0 - Estimator constants

L - Reflux flow rate

L_θ - Logarithmic temperatures based on reference temperatures

$S1 - S3$ - Estimator based on *simulations.*

V - Boilup from reboiler

x_B - Mole fraction of light component in bottom product

y_D - Mole fraction of light component in distillate

y - Output vector $(y_D x_B)^T$

z_F - Mole fraction of light component in feed

Greek symbols

η_M - Murphree tray efficiency

θ - Temperature vector

Θ - Data matrix of θ

Subscripts

c - from calibration set

e - error term

0 - average term

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Chapter 8

Final summary and discussion.

This thesis address the issue of estimating product compositions in distillation columns. The research has been motivated by the large limitations in control performance due to the difficulties both with on-line analyzers and the traditionally temperature control. Distillation columns play an important role in process industry, and better solutions to this problem may give substantial economical savings.

In order to find the most suited estimator for distillation columns, this work started by exploring the general properties of some different approaches.

The most important questions to clarify were

1. The necessary complexity of the estimator, for instance, the loss of performance of using a static estimator compared to a dynamic estimator.

2. The impact of number and types of inputs to the estimator.

3. The impact of noise and uncertainty in measurements and models.

From the literature we chose the classical Kalman filter and the, in process control and for distillation columns, very much cited Brosilow inferential estimator. In addition we found the regression estimator appealing, since it is very simple to implement.

The Structural Singular Value, μ, were chosen as the main tool for performance evaluation of these estimators, because it formed a framework where uncertainty easily could be included, and the need for numerous simulations could be avoided. It also focus the weak spots of the system by always calculating the worst case performance.

The results from tests in this thesis will of course depend somewhat on how we define our system, e.g. how we define the performance and uncertainty weights, and the magnitudes of disturbances etc. However, we believe that the tests are reasonable "fair", that is,

that they includes the most important issues that may affect the estimator performance. However, the tests were performed for just one example column, and the results will not necessarily be valid for all types of columns. However, we think that the example column chosen at least is quite typical for high purity columns.

Main results from the thesis.

Chapter 4.

By including both an "open loop" test and a "closed loop" test, (both estimation and control error test), the following important conclusion can be drawn for the PCR estimator: In spite of substantial estimation error in some frequency ranges, these errors has very little impact on the control performance. We even conclude that the simple regression estimators is preferable to the Kalman filter for the example column. Although the Kalman filter has better open loop performance, the difference in control performance is rather small, and the PCR estimator is much simpler to implement.

These results show that a static estimator might be sufficient for distillation columns. Nonlinear simulations and experimental work confirm this important conclusion. This conclusion has certainly been claimed in the literature before, but an important assumption has not been made clear there: The input to the estimator must consist of temperatures only. The μ-test of the Brosilow estimator shows that including flow measurements, will yield a static estimator with poor performance.

The μ-tests also show that it might be highly questionable to use the input data in *dynamic* estimators as well. This conclusion applies for ill-conditioned plants, where small errors in certain input directions (caused by input gain uncertainty or disturbances) will have large negative impact on the performance. The sensitivity of the estimator for input uncertainty is rarely addressed in the literature. The results should therefore also be viewed as a contribution to highlight this important issue.

Another contribution has been to correct the widespread misconception in the chemical control community that one should delete measurements in order to get a better conditioned estimation problem. The paper shows that one should delete small *directions* in the measurement space rather than the measurements themselves. This may be done by employing for instance PCR or SVD. The use of additional measurements will generally average the measurement noise and for distillation columns yield an estimator with less sensitivity to measurement locations. *Chapter 5* shows that additional measurements may also help to counteract the impact of nonlinearity in the column.

Although simple, PLS and PCR are not completely straight forward methods. For

example, care must be shown in the design of the calibration set to ensure that all important directions are sufficiently exposed. However, the most difficult issue is how to deal with the nonlinearities in high purity columns, i.e. how to obtain a linear estimator that may perform satisfactory in a relative wide range of operating conditions.

Chapter 5 conclude that the nonlinearity may be partly counteracted, by using additional factors. However a better approach is to use logarithmic transformations of the variables. The idea of using logarithmic transforms of temperatures is introduced in this thesis. Since this transform employs differential temperatures it will also give pressure compensation. The benefits of using logarithmic transforms are also confirmed experimentally.

Another approach to improve the estimates is using variable weighting. The results show that the impact of measurement noise should be incorporated in the weight function in addition to the standard deviation. The chapter provides a method for measurement selection based on the weighted temperatures.

This chapter also considers a multicomponent system, and shows that reasonable estimation and control performance can be achieved in this case as well. An important matter dealing with multicomponent systems is to select a reference temperature in the part of the column where the nonkey components have almost flat concentration profiles. The differential temperatures based on these references will then give a kind of non-key compensation in addition to pressure compensation.

In *Chapter 7* the experimental work verifies the usefulness of the logarithmic transforms and weighting. It also shows that an estimator obtained by experimental steady state profiles may yield an estimator with good performance over a wide range of operating conditioned. The need for updating and bias correction was very limited for this estimator.

However, such good data may be very difficult to obtain on an industrial column. Alternatively, one may use an estimator based on simulated calibration runs. The results show that a logarithmic transformed estimator based on simulation runs performs well, as long as the changes operation conditions are relatively small. Some kind of infrequent updating is necessary for this estimator.

Possible improvements and directions for future research.

Even better results may probably be obtained by combining experimental and simulated data. How to perform such a combination, and how to update the estimator are important issues to explore further.

Instead of obtaining a linear calibration estimator, a more rigorous method would be

to use the full nonlinear *static* model of the column. This approach would give more exact estimates, and pitfalls like bad excited calibration sets would be avoided. Luyben and co-workers applied this idea (see Section 3.1.3), but they used basically flow measurements, and only a minimum number of temperatures. However, one would have to use additional measurements to get good results.

The main argument against involving a rigorous nonlinear model is that it is very likely that this approach will give severe computational problems. An on-line routine must of cause guarantee against divergence problems. Whether it is worthwhile to try such a rigorous approach is also a matter of possible improvements in estimate performance. Compared to the PLS and PCR methods they may be relatively small.

In the thesis only product composition estimates are considered. However, a preliminary steady state study indicates that temperatures may be used for feed composition estimates as well. The use of a feed-forward control scheme based on this estimate may perhaps improve the control performance.

There may be situations where a dynamic state observer is preferable and necessary, for example if a predictor is going to be used in the control scheme. Model-predictive control (MPC) and related control schemes have the advantage of including future known setpoints changes in the control action. They explicitely handle hard constraints in the process as well. A comparison of MPC-algorithms with the static PLS-estimator may be an interesting subject for future work.

The temperature measurements, together with other secondary measurement may also be employed for fault detection in distillation columns. Here one could use runs from simulated fault situations as a calibration set to build a simple detection estimator.

Another promising method for better measuring product compositions seems to be on-line Near Infra Red spectroscopy. One drawback with this approach, is that it is not very sensitive for small concentration, and may therefore be difficult to use in the high purity columns. However, this problem is quite analog to that of temperature control. Using tray measurement locations some distance away from the ends could possible extend the application area of this method. Many of the principles of this thesis for temperature estimators might then be employed as well. A combination of temperatures and NIR-measurements may be an even more attractive approach.

Another important task for future work is to gain more experience for the regression estimator with different types of distillation columns. In the theoretical studies a lot of simplification were made, for instant using constant values of relative volatility, tray effi-

ciency and molar flows. The experimental work gave some valuable additional experience, but the extent of that work was nevertheless limited. The binary component system was also rather ideal compared to many systems encountered in industry. The question still remaining, even though the results so fare are very promising, is whether the estimator will prove useful in industry. Experience from implementing the estimator on industrial columns may provide the answer to this question.

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Appendix A

Experimental steady state data.

Data taken during 10 min for Run 1

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	118.7106	0.0218
Temp. tray 1	(°C)	:	117.5057	0.0334
Temp. tray 2	(°C)	:	116.4079	0.0398
Temp. tray 3	(°C)	:	114.1504	0.0775
Temp. tray 4	(°C)	:	109.8088	0.1598
Temp. tray 5	(°C)	:	101.9490	0.2698
Temp. tray 6	(°C)	:	95.8902	0.1621
Temp. tray 7	(°C)	:	88.0099	0.1120
Temp. tray 8	(°C)	:	81.6402	0.0722
Temp. tray 9	(°C)	:	79.1890	0.0372
Temp. tray 10	(°C)	:	77.2144	0.0275
Temp. tray 11	(°C)	:	76.7842	0.0230
Reboiler Level	(Cm)	:	12.6954	0.1539
Accumulator Level	(Cm)	:	11.9891	0.0943
Diff. pressure	(Cm H_2O)	:	30.9018	0.3134
Output signals to actuators:				
Reboiler duty	(Volt)	:	5.0668	0.0706
Distillate pump	(Volt)	:	4.7280	0.0489
Bottom valve	(Volt)	:	8.0087	0.4509
Distillate valve	(Volt)	:	5.5950	0.2037
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.1952	0.012
Bottom composition x_B	(Mol%)	:	0.3713	0.005
Feed composition z_f	(Mol%)	:	45.0212	0.10

Data taken during 10 min for Run 2

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	119.7701	0.0235
Temp. tray 1	(°C)	:	118.2636	0.0435
Temp. tray 2	(°C)	:	116.1904	0.0663
Temp. tray 3	(°C)	:	112.3690	0.1220
Temp. tray 4	(°C)	:	105.8727	0.1668
Temp. tray 5	(°C)	:	97.0548	0.1315
Temp. tray 6	(°C)	:	89.5304	0.1419
Temp. tray 7	(°C)	:	83.5113	0.0782
Temp. tray 8	(°C)	:	80.0423	0.0433
Temp. tray 9	(°C)	:	79.1332	0.0244
Temp. tray 10	(°C)	:	77.9117	0.0230
Temp. tray 11	(°C)	:	77.7446	0.0184
Reboiler Level	(Cm)	:	10.2324	0.2680
Accumulator Level	(Cm)	:	11.9714	0.0959
Diff. pressure	(Cm H_2O)	:	24.6518	0.3788
Output signals to actuators:				
Reboiler duty	(Volt)	:	4.6088	0.1069
Distillate pump	(Volt)	:	4.2506	0.0267
Bottom valve	(Volt)	:	8.0336	0.7832
Distillate valve	(Volt)	:	5.6835	0.2085
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.6350	0.007
Bottom composition x_B	(Mol%)	:	0.6371	0.009
Feed composition z_f	(Mol%)	:	45.7114	0.006

Data taken during 10 min for Run 3

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	119.1208	0.0145
Temp. tray 1	(°C)	:	117.6565	0.0312
Temp. tray 2	(°C)	:	115.7841	0.0498
Temp. tray 3	(°C)	:	112.2051	0.1026
Temp. tray 4	(°C)	:	107.0069	0.1371
Temp. tray 5	(°C)	:	99.4882	0.1676
Temp. tray 6	(°C)	:	92.5084	0.1531
Temp. tray 7	(°C)	:	85.3724	0.0987
Temp. tray 8	(°C)	:	80.5095	0.0516
Temp. tray 9	(°C)	:	79.0260	0.0295
Temp. tray 10	(°C)	:	77.6493	0.0203
Temp. tray 11	(°C)	:	77.5407	0.0123
Reboiler Level	(Cm)	:	7.9115	0.0551
Accumulator Level	(Cm)	:	12.8806	0.1015
Diff. pressure	(Cm H_2O)	:	16.6909	0.0476
Output signals to actuators:				
Reboiler duty	(Volt)	:	3.0499	0.0000
Distillate pump	(Volt)	:	2.4296	0.0337
Bottom valve	(Volt)	:	8.7820	0.1436
Distillate valve	(Volt)	:	5.0953	0.0994
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.6694	0.035
Bottom composition x_B	(Mol%)	:	0.8787	0.013
Feed composition z_f	(Mol%)	:	34.6280	0.035

Data taken during 10 min for Run 4

Measurements:			Average	Stand. dev.
Reboiler Level	(Cm)	:	6.9140	0.0170
Temp. tray 1	(°C)	:	118.4099	0.0204
Temp. tray 2	(°C)	:	117.5784	0.0319
Temp. tray 3	(°C)	:	115.9890	0.0412
Temp. tray 4	(°C)	:	113.7347	0.0833
Temp. tray 5	(°C)	:	108.2402	0.2627
Temp. tray 6	(°C)	:	107.1631	0.0833
Temp. tray 7	(°C)	:	102.5545	0.0862
Temp. tray 8	(°C)	:	94.1451	0.1094
Temp. tray 9	(°C)	:	86.2750	0.0895
Temp. tray 10	(°C)	:	80.4592	0.0477
Temp. tray 11	(°C)	:	78.5636	0.0205
Temp Reboiler	(°C)	:	119.2397	0.0233
Accumulator Level	(Cm)	:	12.1467	0.1476
Diff. pressure	(Cm H_2O)	:	24.0524	0.1706
Output signals to actuators:				
Reboiler duty	(Volt)	:	3.9640	0.0540
Distillate pump	(Volt)	:	3.5428	0.0539
Bottom valve	(Volt)	:	8.4124	0.0853
Distillate valve	(Volt)	:	5.0779	0.0853
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	96.8195	0.0132
Bottom composition x_B	(Mol%)	:	0.1617	0.010
Feed composition z_f	(Mol%)	:	34.3224	0.058

Data taken during 10 min for Run 5

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	120.5731	0.0220
Temp. tray 1	(°C)	:	119.4466	0.0279
Temp. tray 2	(°C)	:	118.4088	0.0257
Temp. tray 3	(°C)	:	116.7508	0.0405
Temp. tray 4	(°C)	:	113.1436	0.1582
Temp. tray 5	(°C)	:	107.8791	0.1959
Temp. tray 6	(°C)	:	99.4420	0.1867
Temp. tray 7	(°C)	:	90.6699	0.1473
Temp. tray 8	(°C)	:	83.0626	0.1238
Temp. tray 9	(°C)	:	80.2326	0.0506
Temp. tray 10	(°C)	:	77.8984	0.0267
Temp. tray 11	(°C)	:	77.3718	0.0192
Reboiler Level	(Cm)	:	7.7118	0.0728
Accumulator Level	(Cm)	:	12.0115	0.0994
Diff. pressure	(Cm H_2O)	:	83.8899	0.7087
Output signals to actuators:				
Reboiler duty	(Volt)	:	8.8216	0.0382
Distillate pump	(Volt)	:	7.7103	0.0141
Bottom valve	(Volt)	:	8.4271	0.2147
Distillate valve	(Volt)	:	5.1680	0.0971
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	98.8059	0.008
Bottom composition x_B	(Mol%)	:	0.1575	0.003
Feed composition z_f	(Mol%)	:	34.5751	0.011

Data taken during 8 min for Run 6

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	119.8009	0.0338
Temp. tray 1	(°C)	:	118.5689	0.0296
Temp. tray 2	(°C)	:	117.4720	0.0299
Temp. tray 3	(°C)	:	115.3521	0.0621
Temp. tray 4	(°C)	:	110.5777	0.1930
Temp. tray 5	(°C)	:	103.9084	0.1998
Temp. tray 6	(°C)	:	94.6654	0.1874
Temp. tray 7	(°C)	:	86.6303	0.1226
Temp. tray 8	(°C)	:	80.9081	0.0614
Temp. tray 9	(°C)	:	78.9508	0.0332
Temp. tray 10	(°C)	:	77.1644	0.0249
Temp. tray 11	(°C)	:	76.8118	0.0297
Reboiler Level	(Cm)	:	6.3719	0.0375
Accumulator Level	(Cm)	:	12.1218	0.1211
Diff. pressure	(Cm H_2O)	:	68.5401	0.2240
Output signals to actuators:				
Reboiler duty	(Volt)	:	8.0060	0.0000
Distillate pump	(Volt)	:	7.4502	0.0240
Bottom valve	(Volt)	:	8.4012	0.1602
Distillate valve	(Volt)	:	5.3467	0.1302
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.1530	0.005
Bottom composition x_B	(Mol%)	:	0.2657	0.013
Feed composition z_f	(Mol%)	:	34.5325	0.012

Data taken during 10 min for Run 7

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	118.0637	0.0274
Temp. tray 1	(°C)	:	116.5353	0.0450
Temp. tray 2	(°C)	:	114.6205	0.0696
Temp. tray 3	(°C)	:	111.0866	0.1122
Temp. tray 4	(°C)	:	106.1335	0.1363
Temp. tray 5	(°C)	:	99.2240	0.1413
Temp. tray 6	(°C)	:	94.6438	0.1732
Temp. tray 7	(°C)	:	88.0976	0.2522
Temp. tray 8	(°C)	:	81.8279	0.1267
Temp. tray 9	(°C)	:	79.1376	0.0519
Temp. tray 10	(°C)	:	77.1478	0.0215
Temp. tray 11	(°C)	:	76.7359	0.0216
Reboiler Level	(Cm)	:	9.1142	0.0146
Accumulator Level	(Cm)	:	12.3385	0.0987
Diff. pressure	(Cm H_2O)	:	13.7681	0.0709
Output signals to actuators:				
Reboiler duty	(Volt)	:	2.4560	0.0000
Distillate pump	(Volt)	:	2.2982	0.0270
Bottom valve	(Volt)	:	8.7811	0.0291
Distillate valve	(Volt)	:	5.0416	0.0957
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.4980	0.002
Bottom composition x_B	(Mol%)	:	0.9534	0.009
Feed composition z_f	(Mol%)	:	34.5325	0.012

Data taken during 8 min for Run 8

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	118.0600	0.0251
Temp. tray 1	(°C)	:	116.3130	0.0432
Temp. tray 2	(°C)	:	114.1973	0.0671
Temp. tray 3	(°C)	:	109.8925	0.1880
Temp. tray 4	(°C)	:	103.3056	0.1320
Temp. tray 5	(°C)	:	95.3015	0.1077
Temp. tray 6	(°C)	:	95.0420	0.0696
Temp. tray 7	(°C)	:	93.6251	0.0630
Temp. tray 8	(°C)	:	90.3434	0.0640
Temp. tray 9	(°C)	:	86.9583	0.0721
Temp. tray 10	(°C)	:	82.1347	0.0650
Temp. tray 11	(°C)	:	78.9255	0.0390
Reboiler Level	(Cm)	:	11.6552	0.0691
Accumulator Level	(Cm)	:	12.0517	0.1026
Diff. pressure	(Cm H_2O)	:	12.9815	0.0621
Output signals to actuators:				
Reboiler duty	(Volt)	:	2.2961	0.0000
Distillate pump	(Volt)	:	2.2237	0.0448
Bottom valve	(Volt)	:	7.4421	0.1127
Distillate valve	(Volt)	:	5.9220	0.0998
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	96.8116	0.0
Bottom composition x_B	(Mol%)	:	1.1048	0.0
Feed composition z_f	(Mol%)	:	54.6133	0.23

Data taken during 10 min for Run 9

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	119.0318	0.0277
Temp. tray 1	(°C)	:	118.0322	0.0319
Temp. tray 2	(°C)	:	117.2418	0.0235
Temp. tray 3	(°C)	:	115.8392	0.0439
Temp. tray 4	(°C)	:	113.0386	0.1451
Temp. tray 5	(°C)	:	107.4998	0.3865
Temp. tray 6	(°C)	:	106.5423	0.1044
Temp. tray 7	(°C)	:	102.9092	0.0880
Temp. tray 8	(°C)	:	95.6881	0.1196
Temp. tray 9	(°C)	:	88.5641	0.1334
Temp. tray 10	(°C)	:	81.2432	0.0710
Temp. tray 11	(°C)	:	78.3191	0.0502
Reboiler Level	(Cm)	:	8.1062	0.0848
Accumulator Level	(Cm)	:	12.0473	0.0911
Diff. pressure	(Cm H_2O)	:	49.0246	0.2875
Output signals to actuators:				
Reboiler duty	(Volt)	:	6.2470	0.0095
Distillate pump	(Volt)	:	5.3283	0.0617
Bottom valve	(Volt)	:	7.5547	0.1091
Distillate valve	(Volt)	:	6.2866	0.0880
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	95.5430	0.0
Bottom composition x_B	(Mol%)	:	0.1103	0.0
Feed composition z_f	(Mol%)	:	54.6133	0.0

Data taken during 8 min for Run 10

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	117.4242	0.0142
Temp. tray 1	(°C)	:	114.7042	0.0699
Temp. tray 2	(°C)	:	110.7779	0.1325
Temp. tray 3	(°C)	:	104.2589	0.2221
Temp. tray 4	(°C)	:	96.9124	0.1663
Temp. tray 5	(°C)	:	90.7225	0.1436
Temp. tray 6	(°C)	:	88.6991	0.0533
Temp. tray 7	(°C)	:	85.5856	0.0609
Temp. tray 8	(°C)	:	81.7902	0.0598
Temp. tray 9	(°C)	:	79.8036	0.0441
Temp. tray 10	(°C)	:	77.5941	0.0308
Temp. tray 11	(°C)	:	76.9087	0.0242
Reboiler Level	(Cm)	:	9.3011	0.0430
Accumulator Level	(Cm)	:	12.2172	0.0659
Diff. pressure	(Cm H_2O)	:	14.8465	0.1082
Output signals to actuators:				
Reboiler duty	(Volt)	:	2.8879	0.0000
Distillate pump	(Volt)	:	2.3181	0.0339
Bottom valve	(Volt)	:	8.4438	0.0579
Distillate valve	(Volt)	:	6.2695	0.0609
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.1007	0.0
Bottom composition x_B	(Mol%)	:	2.6616	0.0
Feed composition z_f	(Mol%)	:	54.3574	0.0

Data taken during 8 min for Run 11

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	119.2820	0.1750
Temp. tray 1	(°C)	:	118.1958	0.0392
Temp. tray 2	(°C)	:	117.0935	0.0245
Temp. tray 3	(°C)	:	115.0797	0.0642
Temp. tray 4	(°C)	:	110.2600	0.1722
Temp. tray 5	(°C)	:	103.4164	0.2990
Temp. tray 6	(°C)	:	94.6442	0.2124
Temp. tray 7	(°C)	:	86.6701	0.1739
Temp. tray 8	(°C)	:	80.6245	0.0985
Temp. tray 9	(°C)	:	78.5017	0.0427
Temp. tray 10	(°C)	:	76.5798	0.0222
Temp. tray 11	(°C)	:	76.1866	0.0205
Reboiler Level	(Cm)	:	7.7216	0.0618
Accumulator Level	(Cm)	:	12.3898	0.1227
Diff. pressure	(Cm H_2O)	:	60.2642	0.1862
Output signals to actuators:				
Reboiler duty	(Volt)	:	8.3749	0.0000
Distillate pump	(Volt)	:	7.6630	0.0432
Bottom valve	(Volt)	:	6.4099	0.0947
Distillate valve	(Volt)	:	5.5466	0.1292
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.1275	0.0
Bottom composition x_B	(Mol%)	:	0.2215	0.0
Feed composition z_f	(Mol%)	:	55.2762	0.0

Data taken during 8 min for Run 12

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	116.9290	0.0088
Temp. tray 1	(°C)	:	114.6895	0.0542
Temp. tray 2	(°C)	:	111.2956	0.0972
Temp. tray 3	(°C)	:	105.2364	0.1648
Temp. tray 4	(°C)	:	97.9585	0.1482
Temp. tray 5	(°C)	:	90.9828	0.1432
Temp. tray 6	(°C)	:	88.5562	0.0505
Temp. tray 7	(°C)	:	84.8269	0.0510
Temp. tray 8	(°C)	:	80.7646	0.0525
Temp. tray 9	(°C)	:	78.7793	0.0314
Temp. tray 10	(°C)	:	76.7647	0.0213
Temp. tray 11	(°C)	:	76.1306	0.0155
Reboiler Level	(Cm)	:	6.7539	0.0573
Accumulator Level	(Cm)	:	13.2422	0.0616
Diff. pressure	(Cm H_2O)	:	5.3861	0.1169
Output signals to actuators:				
Reboiler duty	(Volt)	:	2.9620	0.0486
Distillate pump	(Volt)	:	2.9411	0.0234
Bottom valve	(Volt)	:	7.9444	0.2053
Distillate valve	(Volt)	:	6.1934	0.0597
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.2696	0.0
Bottom composition x_B	(Mol%)	:	2.1758	0.0
Feed composition z_f	(Mol%)	:	55.5999	0.0

Data taken during 10 min for Run 13

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	117.3782	0.0370
Temp. tray 1	(°C)	:	116.4614	0.0278
Temp. tray 2	(°C)	:	115.3909	0.0341
Temp. tray 3	(°C)	:	113.1179	0.0852
Temp. tray 4	(°C)	:	109.2585	0.1728
Temp. tray 5	(°C)	:	101.6148	0.3884
Temp. tray 6	(°C)	:	97.6285	0.2145
Temp. tray 7	(°C)	:	90.5700	0.1829
Temp. tray 8	(°C)	:	82.9688	0.1196
Temp. tray 9	(°C)	:	79.2094	0.0611
Temp. tray 10	(°C)	:	76.5135	0.0372
Temp. tray 11	(°C)	:	75.8429	0.0401
Reboiler Level	(Cm)	:	7.4824	0.0831
Accumulator Level	(Cm)	:	11.7970	0.1160
Diff. pressure	(Cm H_2O)	:	26.0508	0.2251
Output signals to actuators:				
Reboiler duty	(Volt)	:	4.6052	0.0322
Distillate pump	(Volt)	:	4.5858	0.0353
Bottom valve	(Volt)	:	8.0328	0.1020
Distillate valve	(Volt)	:	5.4723	0.1140
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.0091	0.0
Bottom composition x_B	(Mol%)	:	0.3588	0.0
Feed composition z_f	(Mol%)	:	50.7911	0.0

Data taken during 6 min for Run 14

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	118.1077	0.0189
Temp. tray 1	(°C)	:	117.0919	0.0316
Temp. tray 2	(°C)	:	116.1711	0.0305
Temp. tray 3	(°C)	:	114.4482	0.0557
Temp. tray 4	(°C)	:	110.7948	0.1580
Temp. tray 5	(°C)	:	103.6304	0.4031
Temp. tray 6	(°C)	:	101.5202	0.1093
Temp. tray 7	(°C)	:	96.1429	0.0908
Temp. tray 8	(°C)	:	88.2151	0.0979
Temp. tray 9	(°C)	:	82.6177	0.0751
Temp. tray 10	(°C)	:	78.1987	0.0414
Temp. tray 11	(°C)	:	76.7576	0.0194
Reboiler Level	(Cm)	:	8.4560	0.0613
Accumulator Level	(Cm)	:	11.8353	0.1010
Diff. pressure	(Cm H_2O)	:	40.4861	0.1991
Output signals to actuators:				
Reboiler duty	(Volt)	:	5.8836	0.0953
Distillate pump	(Volt)	:	5.4169	0.0343
Bottom valve	(Volt)	:	7.5867	0.1824
Distillate valve	(Volt)	:	6.2904	0.0983
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	97.7121	0.0
Bottom composition x_B	(Mol%)	:	0.2187	0.0
Feed composition z_f	(Mol%)	:	54.3241	0.0

Data taken during 10 min for Run 13

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	117.3782	0.0370
Temp. tray 1	(°C)	:	116.4614	0.0278
Temp. tray 2	(°C)	:	115.3909	0.0341
Temp. tray 3	(°C)	:	113.1179	0.0852
Temp. tray 4	(°C)	:	109.2585	0.1728
Temp. tray 5	(°C)	:	101.6148	0.3884
Temp. tray 6	(°C)	:	97.6285	0.2145
Temp. tray 7	(°C)	:	90.5700	0.1829
Temp. tray 8	(°C)	:	82.9688	0.1196
Temp. tray 9	(°C)	:	79.2094	0.0611
Temp. tray 10	(°C)	:	76.5135	0.0372
Temp. tray 11	(°C)	:	75.8429	0.0401
Reboiler Level	(Cm)	:	7.4824	0.0831
Accumulator Level	(Cm)	:	11.7970	0.1160
Diff. pressure	(Cm H_2O)	:	26.0508	0.2251
Output signals to actuators:				
Reboiler duty	(Volt)	:	4.6052	0.0322
Distillate pump	(Volt)	:	4.5858	0.0353
Bottom valve	(Volt)	:	8.0328	0.1020
Distillate valve	(Volt)	:	5.4723	0.1140
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.0091	0.0
Bottom composition x_B	(Mol%)	:	0.3588	0.0
Feed composition z_f	(Mol%)	:	50.7911	0.0

Data taken during 6 min for Run 14

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	118.1077	0.0189
Temp. tray 1	(°C)	:	117.0919	0.0316
Temp. tray 2	(°C)	:	116.1711	0.0305
Temp. tray 3	(°C)	:	114.4482	0.0557
Temp. tray 4	(°C)	:	110.7948	0.1580
Temp. tray 5	(°C)	:	103.6304	0.4031
Temp. tray 6	(°C)	:	101.5202	0.1093
Temp. tray 7	(°C)	:	96.1429	0.0908
Temp. tray 8	(°C)	:	88.2151	0.0979
Temp. tray 9	(°C)	:	82.6177	0.0751
Temp. tray 10	(°C)	:	78.1987	0.0414
Temp. tray 11	(°C)	:	76.7576	0.0194
Reboiler Level	(Cm)	:	8.4560	0.0613
Accumulator Level	(Cm)	:	11.8353	0.1010
Diff. pressure	(Cm H_2O)	:	40.4861	0.1991
Output signals to actuators:				
Reboiler duty	(Volt)	:	5.8836	0.0953
Distillate pump	(Volt)	:	5.4169	0.0343
Bottom valve	(Volt)	:	7.5867	0.1824
Distillate valve	(Volt)	:	6.2904	0.0983
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	97.7121	0.0
Bottom composition x_B	(Mol%)	:	0.2187	0.0
Feed composition z_f	(Mol%)	:	54.3241	0.0

	Stand.
ge	dev.
1	0.0206
1	0.0216
2	0.0279
3	0.0645
5	0.1223
4	0.2531
7	0.1724
5	0.1932
9	0.1522
7	0.0632
5	0.0248
4	0.0115
8	0.0207
7	0.1238
0	0.1021
9	0.0192
6	0.0436
7	0.0373
3	0.1087
0	0.0
0	0.0
4	0.0

Data taken during 9 min for Run 16

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	119.4909	0.0108
Temp. tray 1	(°C)	:	118.5821	0.0167
Temp. tray 2	(°C)	:	117.6307	0.0225
Temp. tray 3	(°C)	:	116.0574	0.0637
Temp. tray 4	(°C)	:	112.6562	0.1719
Temp. tray 5	(°C)	:	106.1199	0.1796
Temp. tray 6	(°C)	:	98.7210	0.1875
Temp. tray 7	(°C)	:	90.1314	0.1538
Temp. tray 8	(°C)	:	82.6873	0.0974
Temp. tray 9	(°C)	:	79.9062	0.0427
Temp. tray 10	(°C)	:	77.6835	0.0245
Temp. tray 11	(°C)	:	77.1810	0.0120
Reboiler Level	(Cm)	:	8.3206	0.0467
Accumulator Level	(Cm)	:	10.9759	0.1178
Diff. pressure	(Cm H_2O)	:	47.3977	0.2413
Output signals to actuators:				
Reboiler duty	(Volt)	:	6.5591	0.0264
Distillate pump	(Volt)	:	6.1109	0.0288
Bottom valve	(Volt)	:	7.1673	0.1791
Distillate valve	(Volt)	:	4.9173	0.1412
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.137	0.0
Bottom composition x_B	(Mol%)	:	0.253	0.0
Feed composition z_f	(Mol%)	:	42.95	0.0

Data taken during 10 min for Run 17

Measurements:			Average	Stand. dev.
Temp Reboiler	(°C)	:	117.7772	0.0169
Temp. tray 1	(°C)	:	116.8447	0.0282
Temp. tray 2	(°C)	:	115.6590	0.0324
Temp. tray 3	(°C)	:	113.3402	0.0649
Temp. tray 4	(°C)	:	109.3144	0.1421
Temp. tray 5	(°C)	:	101.4459	0.2443
Temp. tray 6	(°C)	:	95.8662	0.1808
Temp. tray 7	(°C)	:	87.7973	0.1723
Temp. tray 8	(°C)	:	81.1274	0.0998
Temp. tray 9	(°C)	:	78.5457	0.0452
Temp. tray 10	(°C)	:	76.5404	0.0192
Temp. tray 11	(°C)	:	76.1441	0.0103
Reboiler Level	(Cm)	:	7.5826	0.0507
Accumulator Level	(Cm)	:	23.2305	0.1161
Diff. pressure	(Cm H_2O)	:	26.3798	0.0782
Output signals to actuators:				
Reboiler duty	(Volt)	:	4.0462	0.0172
Distillate pump	(Volt)	:	4.0510	0.0486
Bottom valve	(Volt)	:	7.3448	0.1529
Distillate valve	(Volt)	:	5.0378	0.1980
Gas Chromatograph analysis:				
Top composition y_D	(Mol%)	:	99.415	0.0
Bottom composition x_B	(Mol%)	:	0.330	0.0
Feed composition z_f	(Mol%)	:	45.700	0.0