

# Self-Optimizing Control of the Kaibel Distillation Column

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December 19, 2005

### **Abstract**

The minimum singular value method for finding optimal controlled variables is introduced. The method is applied to control structure design for a four-product Kaibel distillation column, which is a mass and heat integrated separation column. The selection method is based on steady-state optimization. It is shown how this can be done, using the commercial process simulator Hysys v3.2.

**KEYWORDS** : Control Structure Design, Optimization, Convexity.

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# Preface

This report is the culmination of my project work, as part of the specialization in process systems engineering at the Department of Chemical Engineering at the Norwegian University of Science and Technology (NTNU).

The aim of the project was to find a self-optimizing control structure for the Kaibel distillation column, which is a column with a dividing wall, which makes it possible to separate up to four components in one column shell.

# Chapter 1

## Background

### 1.1 The Kaibel Distillation Column

The Kaibel distillation column was introduced by Gerd Kaibel at BASF in 1987. The Kaibel column is a heat and mass integrated separation process, with potential for large savings in capital cost, energy requirement and plot space compared to the conventional sequential distillation for multicomponent separations. In sequential distillation one needs three columns to separate four components. Up to 40% savings in plot space has been reported, and up to 25% and 35% respectively for investment and operating cost [Wenzel and Röhm, 2003].

Heat and mass integration can be achieved both in a dividing-wall implementation and when the prefractionator and main tower are built in separate shells. A laboratory column has been built at the Department of Chemical Engineering, NTNU, to do pilot plant experiments, and this column has been built with two shells. This would not be the best solution in an industrial application, when investment costs are important, but the energy savings will be the same, assuming adiabatic operation.

A conceptual model of the Kaibel column is shown in figure 1.1. On the left hand side, the prefractionator is shown, where the 4-component mixture is split into two fractions; one light and one heavy. On the right hand side, the main separation tower is shown, where the two fractions are split into their respective components. There is only one reboiler and one condenser for such a column.

BASF has implemented several dividing-wall columns in production scale. A simulation structure for design of such columns is given by Kaibel [Kaibel et al., 2004]. Kaibel also mentions the control of such columns at BASF, and the control objective is most often to maintain the product balance (steady-state operation) and the given quality constraints. The control loops at BASF are designed and implemented without dynamic simulations.

For the control of the column, there are 6 steady-state degrees of free-

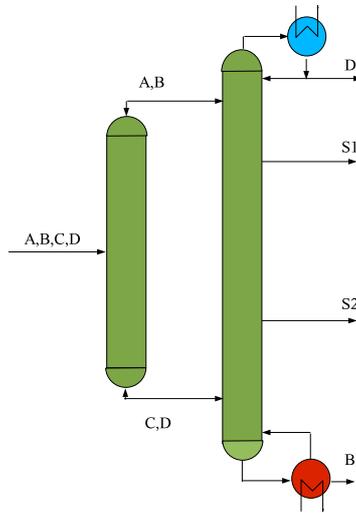


Figure 1.1: Schematic of a Kaibel distillation column

dom: reflux and boil-up, splits of internal streams and two product streams. In the analysis to follow, two of these (boil-up and vapor split) are kept constant, and the remaining 4 degrees of freedom are available to the control system. The simulation is based on molar flows, but the real system will be controlled based on volume flow. Assuming a nearly constant composition profile (molar mass profile), these are one-to-one related variables.

## 1.2 The Physics of Distillation

The separating agent in distillation is energy, supplied to the distillation column in the reboiler. Continuous distillation is a staged separation process, and vapor and liquid phases are contacted at each stage, where equimolar diffusion occurs. The driving forces for the diffusion are entropic in nature, and with sufficient contact time and interface between the phases will eventually reach equilibrium at each stage. In real distillations the process is not at equilibrium, but the equilibrium model serves as a good conceptual model for understanding the behavior of the distillation process. The underlying assumption is that two un-equilibrated streams entering a typical stage, have a residence time at the stage which is much larger than the necessary contact time for equilibrium to be reached through diffusion.

For control purposes it is interesting to know how different manipulable variables affect the process. First of all, the measurements normally accessible to control are temperature measurements. The temperature profile of a distillation column is coupled to the concentration profile through the thermodynamics. Concentrations are hard to measure directly, and the mea-

surement is slow. The link between the temperature measurements and the product concentrations is established as an empirical model.

The pressure in a distillation column is set such that the condenser and reboiler can work with the utilities available. In most cases the pressure is kept constant (often atmospheric), but it can also be a controllable property. This can be practical for example when operating close to the utility constraints, because of changes in ambient temperature. Increasing the pressure increases the condenser temperature, but at the same time the reboiler temperature increases.

### 1.2.1 The Effect Changing the Flow Inputs

Often in distillation, the internal flows, reflux and boil-up, are used as control degrees of freedom. In a two-product multicomponent distillation column, the effect of changing an internal flow on the concentration profile is to move the whole profile; one product tends to get purer, whereas the other gets less pure [Skogestad, 1997]. However, the effect of changing the external flows is much larger, if one draws a lot more in the top stream as there is light component in the feed, it is obvious that the product purity will be lower. The use of external streams as controlled variables is limited, because they are often needed in order to stabilize levels in the reboiler and reflux drum.

## 1.3 Self-Optimizing Control

When operating a chemical process, there is usually some optimal operating point, and it is economically imperative to stay close to this operating point. This point is however dependent on process conditions, and may move in the state-space due to disturbances on the process. The primary control objective is related to profits, and thus the selection of controlled variables should reflect this. In other words; the selection of the best control structure is a question of optimization; a structure should be selected so that the loss,  $L = J(u, d) - J^*(d)$  is minimized, where  $J$  is an objective function describing the operational objective, and  $J^*(d)$  is the optimum for a given disturbance  $d$ .

Skogestad and Postlethwaite [Skogestad and Postlethwaite, 2005] define the concept of self-optimizing control the following way:

**Definition 1 (Self-Optimizing Control)** *Self-optimizing control is when an acceptable loss can be achieved with constant set-points, without the need for reoptimization when disturbances occur.*

### 1.3.1 Selection of controlled outputs

The method used for selecting optimal controlled variables is a local optimization method. The loss is defined as above. Make the following assump-

tions:

- the cost function  $J$  is smooth.
- the optimization problem is unconstrained, i.e., active constraints are already controlled at their optimal values.
- the dynamics of the process can be neglected when evaluating the cost.
- the control problem is square (the number of controlled outputs equals the number of manipulated variables).

Then, a second order approximation to the objective function is made by a Taylor expansion around the optimal operating point (where  $\Delta u = u - u^*$ , etc.):

$$J(u, d) = J^*(d) + (\nabla_u J^*)^T \Delta u + \frac{1}{2} (\Delta u)^T (\nabla_u^2 J^*) \Delta u \quad (1.1)$$

Then, the loss can be written the following way:

$$L = J(u, d) - J^*(d) = \frac{1}{2} (\Delta u)^T (\nabla_u^2 J^*) \Delta u \quad (1.2)$$

To analyze how the loss inflicted on the objective function by the non-optimal inputs  $\Delta u$  affects the output selection, assume a steady-state linear model is available,

$$z = Gu + G_d d \quad (1.3)$$

where  $G$  and  $G_d$  are steady-state gain matrices for the inputs and disturbances respectively. Assuming that  $G$  is non-singular and focusing on the input-output behavior:

$$\Delta u = G^{-1} \Delta z \quad (1.4)$$

Equation (1.4) together with (1.2) yields

$$L = \frac{1}{2} (G^{-1} \Delta z)^T (\nabla_u^2 J) (G^{-1} \Delta z) = \frac{1}{2} (\Delta z)^T G^{-T} J_{uu} (G^{-1} \Delta z) \quad (1.5)$$

Now, defining a mapping of  $z$  through the loss model;

$$\tilde{z} := J_{uu}^{1/2} G^{-1} \Delta z \quad (1.6)$$

The loss minimization can be expressed as a norm minimization problem;

$$L = \frac{1}{2} \|\tilde{z}\|_2^2 \quad (1.7)$$

The control error can be separated in two terms; the implementation error and the optimization error due to the non-optimal operating point. The

optimization error can be estimated as the worst-case variation in solutions to the optimization problem with varying disturbances. Let  $r$  be the reference point for the controlled variable  $z$ . Then the error can be expressed:

$$e = z - z^* = \underbrace{z - r}_I + \underbrace{r - z^*}_{e_{opt}} \quad (1.8)$$

where  $I$  is the implementation error and  $e_{opt}$  the optimization error. With integral action in the controller, there is no setpoint tracking error, and the implementation error is basically the measurement error.

From (1.5), it is easily seen that, to obtain good control, one should seek controlled variables such that:

- $G^{-1}$  is small, that is, the gain should be high.
- $e_{opt}$  should be small;  $z_{opt}$  should be insensitive to disturbances.
- $G$  should be well conditioned.

## MIMO Systems: Minimum Singular Value

Assume that the optimal variation in the outputs is uncorrelated, that is, the worst-case deviation  $\|z - z^*\| = 1$  can occur. Assume also that the inputs are scaled such that a given deviation  $\Delta u_i$  has a similar effect on the cost function  $J$  for all inputs, that is, the Hessian is a constant  $\alpha$  times a unitary matrix, where  $\alpha = \bar{\sigma}(J_{uu})$ . Then the norm of the augmented error,  $\tilde{z}$ , is  $\|\tilde{z}\| = \bar{\sigma}(J_{uu}^{1/2} G^{-1})$ , and the worst-case loss is;

$$\max_{\|z - z^*\| \leq 1} L = \frac{1}{2} \bar{\sigma}^2(\alpha^2 G^{-1}) = \frac{\alpha}{2} \frac{1}{\underline{\sigma}^2(G)} \quad (1.9)$$

From equation (1.9) it is apparent that controlled variables should be chosen to maximize the minimum singular value.

## 1.4 Mathematical Background

### 1.4.1 Convexity

Convexity is a very important property of an optimization problem. A scalar-valued function is convex in a point if its second derivative in the point is positive. If this holds for all points in the domain of the function, the function is itself called convex. A minimizer for a convex function is a global minimizer, because there exists a unique minimum. An example of a convex function is shown in figure 1.2. A non-convex function is shown in figure 1.3, such a function may have several minima, and the global one is therefore hard to find.

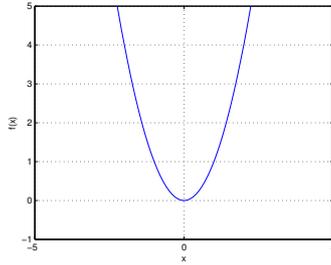


Figure 1.2: A convex function

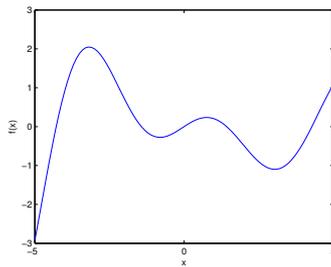


Figure 1.3: A non-convex function

### 1.4.2 A Formal Definition of Convexity

**Definition 2 (Convex Set)** A set  $S \in \mathbb{R}^n$  is called convex if a straight line segment connecting any two points in  $S$  lies entirely within  $S$ . Formally, for any two points  $(x, y) \in S$ :  $\alpha x + (1 - \alpha)y \in S, \forall \alpha \in [0, 1]$ .

**Definition 3 (Convex Function)** A function  $f$  is called convex if its domain is a convex set as defined in definition 2, and if for any two points  $(x, y)$  in the domain of  $f$ , the graph of  $f$  lies below the straight line connecting  $(x, f(x))$  to  $(y, f(y))$  in the  $(n+1)$ -dimensional space  $\mathbb{R}^{n+1}$ . That is, we have  $\forall \alpha \in [0, 1]$ :

$$f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y)$$

### Convex Programming

Convex programming is a term used for the solution of a special class of constrained optimization problems, where the objective function is convex, the equality constraints are linear and the inequality constraints are concave. This is usually not the case in process optimization, because the thermodynamic equilibrium is mostly described by nonlinear functions, and these are then equality constraints for the optimization problem.

### 1.4.3 Numerical Optimization Algorithms

The optimization methods utilized in this work are local. The most popular class of local optimization methods is the quasi-Newton approach. Assume we have an unconstrained nonlinear problem. For the quasi-Newton approach, this objective function  $J(p)$  is approximated by a quadratic function  $m_k(p)$ , where  $p$  is the vector of free variables.  $J$  is assumed to be a real-valued scalar function. The quadratic approximation is given by;

$$m_k(p) = J_k + \nabla J_k^T p + \frac{1}{2} p^T B_k p \quad (1.10)$$

where  $B$  is some positive definite matrix, which is updated on every iteration. This model is convex and quadratic, and its minimizer,  $p_k$  can be given explicitly as;

$$p_k = -B_k^{-1} \nabla J_k \quad (1.11)$$

The minimizer given in (1.11) is used as the search direction, and the new iterate is then

$$x_{k+1} = x_k + \alpha_k p_k \quad (1.12)$$

where the step length must satisfy the Wolfe conditions. The Wolfe conditions guarantee a step length that yields sufficient decrease of the objective function, assuming convexity. The following must be fulfilled:

$$\begin{aligned} J(x_k + \alpha_k p_k) &\leq J(x_k) + c_1 \alpha_k \nabla J_k^T p_k \\ \nabla J(x_k + \alpha_k p_k)^T &\geq c_2 \nabla J_k^T p_k \end{aligned}$$

where  $0 < c_1 < c_2 < 1$ . The difference between this method and an exact Newton method, is that an approximation of the Hessian is used instead of the true one.

The update formula for the Hessian approximation should satisfy some important criteria: it must be positive definite and symmetric. One of the most popular update formulas, is the BFGS formula, here simply stated for reference.<sup>1</sup> For details about the BFGS update, see [Nocedal and Wright, 1999]. For convenience of notation the following vectors are defined:

$$s_k := x_{k+1} - x_k \quad (1.13)$$

$$y_k := \nabla J_{k+1} - \nabla J_k \quad (1.14)$$

Then the BFGS formula can be written as:

$$H_{k+1} = (I - \rho_k s_k y_k^T) H_k (I - \rho_k y_k s_k^T) + \rho_k s_k s_k^T \quad (1.15)$$

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<sup>1</sup>BFGS is an abbreviation for Broyden, Fletcher, Goldfarb and Shanno, the discoverers of the formula

where  $\rho = \frac{1}{y_k^T s_k}$  and  $H_k$  is the inverse of the Hessian approximation:

$$H_k = B_k^{-1}$$

The quasi-Newton BFGS method applies directly only to unconstrained problems. In process optimization, the process model poses a large set of equality constraints on the problem, whereby many equations are nonlinear. The equality constraints of the process model must be taken into the objective function, because they limit the allowable domain of the problem to a subset of the natural domain of the objective function, called the feasible set,  $\Omega$ . The constraints are brought into the objective function by forming the Lagrangian, and then for solving the problem a search routine as for unconstrained optimization can be used. If there are inequality constraints, the active set method is used. Inequality constraints in process optimization are often constraints on quality and availability.

For general nonlinear constrained optimization, the Karush-Kuhn-Tucker conditions are necessary for characterization of a local minimizer. Assuming the linear independence constraint qualification (LICQ) is fulfilled:

**Definition 4 (Linear Independence Constraint Qualification)** *Given the point  $x^*$  and the active set  $\mathcal{A}(x^*)$ , which is the set defined by the equality constraints and the active inequality constraints, the linear independence constraint qualification holds if the set of active constraint gradients is linearly independent. This set is then:*

$$\{\nabla c_i(x^*), i \in \mathcal{A}(x^*)\}$$

If the linear independence constraint qualification holds, then the KKT conditions can be stated as necessary conditions for a local optimum:

**Definition 5 (KKT conditions)** *Suppose  $x^*$  is a solution to the optimization problem. Then there is a Lagrange multiplier vector  $\lambda^*$  with components  $\lambda_i^*$  with  $i \in I = I_{in} \cup I_{eq}$ , such that the following conditions are satisfied at  $p = (x^*, \lambda^*)$ :*

$$\nabla_x \mathcal{L}(p) = 0 \tag{1.16}$$

$$c_i(x^*) = 0 \forall i \in I_{eq} \tag{1.17}$$

$$c_i(x^*) \geq 0, \forall i \in I_{in} \tag{1.18}$$

$$\lambda_i^* \geq 0, \forall i \in I_{in} \tag{1.19}$$

$$\lambda_i^* c_i(x^*) = 0 \forall i \in I \tag{1.20}$$

In order to test for optimality, a routine also needs information about the curvature of the objective function around the stationary point. It is sufficient that the second derivative is strictly positive and that the KKT first-order conditions are satisfied.

For the multivariable case, the second-derivative condition is that the Hessian must be positive definite. For details, see [Nocedal and Wright, 1999].

## 1.5 Computational Issues

The process model is implemented in Hysys v3.2., which is a process simulator from AspenTech, and the optimizer in this program is also used for the optimization tasks. The selection of the best candidates for control variables is done using a branch and bound method implemented in MATLAB 7.1. Therefore, it is of interest to export the simulation results from Hysys to MATLAB. This is however not too easily done, and it is also of interest to have a simple visual data storage format. The solution was to export all results from Hysys to Excel, which can be easily done, using Hysys reports, which can be exported as comma separated ASCII files, which Excel again can convert to a spreadsheet workbook. MATLAB has functions for extracting parts of a spreadsheet, and storing them as matrices in the workspace. MATLAB can also write to specified portions of Excel spreadsheets, so this seemed the most appropriate storage tool in this case. Excel was also used for calculating the gain matrix and scaling factors. For details on software connectivity and the versions used, see appendix B

It is also interesting to visualize solutions to the optimization problems. This requires a lot of calculations in Hysys, which would be a tedious task without automation. Hysys has a good application programming interface for integration with Visual Basic, which is the macro language in MS Office. This means, that Hysys can be used as an automated calculation engine for Excel, and Excel can then be used to calculate data points for sensitivity plots.

### 1.5.1 Distillation Models

Distillation models can be divided into two main classes:

- Equilibrium stage models
- Mass transfer models

The most common models for distillation design and simulation are of the first class, where the process is assumed to consist of equilibrium stages, and empirical correction factors are used to account for the fact that true equilibrium is usually not reached.

The model used by Hysys is of the equilibrium kind. Plate efficiencies can be used in the simulation to account for the difference between ideal equilibrium stages and real plates in a plate tower. The steady-state model consists of the component mass balances, the energy balance, summation equations and a model for the phase equilibrium. For one stage  $j$ , the model can be written as follows:

$$L_{j-1} - L_j + V_{j+1} - V_j + F_j - R_j = 0 \quad (1.21)$$

$$x_{i,j-1}L_{j-1} - x_{i,j}L_j + y_{i,j+1}V_{j+1} - y_{i,j}V_j + z_{i,j}F_j - x_{i,j}R_j = 0 \quad (1.22)$$

$$\sum_i x_{i,j} = 1 \quad (1.23)$$

$$\sum_i y_{i,j} = 1 \quad (1.24)$$

$$h_{j-1}^L L_{j-1} - h_j^L L_j + h_{j+1}^V V_{j+1} - h_j^V V_j + h_{F_j} F - h_j^L R_j = 0 \quad (1.25)$$

$$y_{i,j} = K_{i,j} x_{i,j} \quad (1.26)$$

where  $x_{i,j}$  is the mole fraction of component  $i$  in the liquid phase on stage  $j$ . It is assumed that only liquid will be withdrawn from the stage, product streams are denoted  $R_j$ .  $F_j$  is the feed and  $z_{i,j}$  is the mole fraction of component  $i$  in the feed to stage  $j$ .  $h_j^\phi$  is the molar enthalpy of phase  $\phi$  on stage  $j$ . The equilibrium is described through the equilibrium constant  $K_{i,j}$ , which is calculated using some model for the non-ideal behavior of the system. The K-value is what introduces the strongest non-linear terms in a steady-state distillation model. Note that the terms  $F_j$  and  $R_j$  are zero for most stages.

In addition to the equilibrium stages, the Kaibel column is modeled with two internal splitters. These are described by simple material balances. In addition there are also a reboiler and a condenser, which are modeled using the same equations as for equilibrium stages, but with an extra energy term  $Q$ , which is positive for the reboiler and negative for the condenser (heat removed).

### 1.5.2 Thermodynamic Models

The thermodynamic relationship to use for the  $K$ -value calculation must be chosen such that the model is able to model the non-ideal behavior of the system well. Alcohols are polar substances, and thus some activity model should be used. For low molecular weight alcohols like methanol and ethanol, the Wilson local composition theory has been shown to have good properties.

Assuming ideal gas behavior of the vapor phase, which is reasonable at low pressures, and an activity model for the liquid phase, the equilibrium can be expressed as in (1.27). There the approximation  $f_i \approx P_i^{sat}$  is included,  $f_i$

being the pure component liquid fugacity,  $f_i$  being the pure component liquid fugacity.

$$y_i P = x_i \gamma_i P_i^{sat} \quad (1.27)$$

Here,  $\gamma_i$  is the activity coefficient and  $P_i^{sat}$  is the vapor pressure of pure component  $i$ . Then the  $K$ -value can be introduced as  $K_i = y_i/x_i = \gamma_i P_i^{sat}/P$ . The vapor pressure can be calculated using the Antoine equation. The activity coefficient must be calculated using some activity model. In Wilson's model, the expression for the activity coefficient is given by [Elliot and Lira, 1999]:

$$\ln \gamma_k = 1 - \ln \left( \sum_i x_i \Lambda_{ki} \right) - \sum_j \left( \frac{x_j \Lambda_{jk}}{\sum_i x_i \Lambda_{ji}} \right) \quad (1.28)$$

Here,  $\Lambda_{jk}$  is a binary interaction parameter depending on molecular volumes and temperature.

## Chapter 2

# Control Structure Selection

The selection of controlled variables is done using the minimum singular value rule, as described in 1.3.1 and a steady-state model in Hysys.

### 2.1 Model of the Kaibel Column

A model of the column was implemented in Hysys for steady-state simulation and optimization. The model structure is shown in figure 2.1.

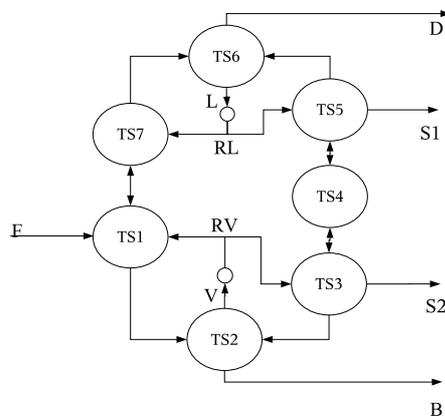


Figure 2.1: Structure of the internal Kaibel model in Hysys

This is built using the column subflowsheet in Hysys, and stored as a unit operation template which can be used as any other unit operation in Hysys simulations. To have splitters and other non-standard internals in the column model, a special algorithm called *Modified HYSIM Inside-Out* must be used to solve the steady-state problem.

## 2.2 Nominal Operating Point

To find the nominal operating point, sensible start values must be given. These are chosen from [Strandberg and Skogestad, 2005]. The start values for finding the optimal nominal operating point are as given in Table 2.1.

Variable	Magnitude	Unit
$R_L, R_V$	0.3	–
$S_1, S_2$	0.25	kmol/h
$V, L$	3	kmol/h

Table 2.1: Start values for optimization

The objective is to produce the purest products possible. Let  $i$  be the index of product stream ( $i=1: D, i=2: S_1, \dots$ ) and  $j$  be the index of a component ( $j=1: C-1, j=2: C-2, \dots$ ). Then this objective can be described by the following cost function:

$$J = \sum_{i=1}^4 \sum_{j=1|j \neq i}^4 x_{ij} \quad (2.1)$$

The start values from Table 2.1 yield a cost function value of  $J = 0.77$ , which is not very high degree of purity. An optimization with six degrees of freedom yields  $J = 0.1299$ . The nominal case is summarized in Table 2.2.

Variable	Magnitude	Unit
$R_L$	0.2668	–
$R_V$	0.4561	–
$L$	2.982	kmol/h
$V$	3.052	kmol/h
$S_1$	0.2517	kmol/h
$S_2$	0.2488	kmol/h
$J$	0.1299	–

Table 2.2: Optimal values for nominal situation

### 2.2.1 Characterization of the Optimization Problem

Visualization of the optimum gives a qualitative insight into the problem at hand. A sensitivity study was performed for characterizing the optimum. The process variables affect the purity, and this comes into the optimization problem as equality constraints. There are 64 stages in the model, plus two splitters, and a reboiler and a condenser. For each stage the material balance, energy balance and equilibrium relations must be satisfied. This

gives some hundred equality constraints on the optimization problem, and many of these are non-linear. These equality constraints are taken into consideration through the lagrangian. Using a quasi-Newton method, this multivariable non-linear cost function is approximated by a second-order polynomial function.

## Visualization of the Cost Function

The sensitivity study shows that the cost function resembles a quadratic dependency on the side draws  $S_1$  and  $S_2$ , see figures 2.2 and 2.3.

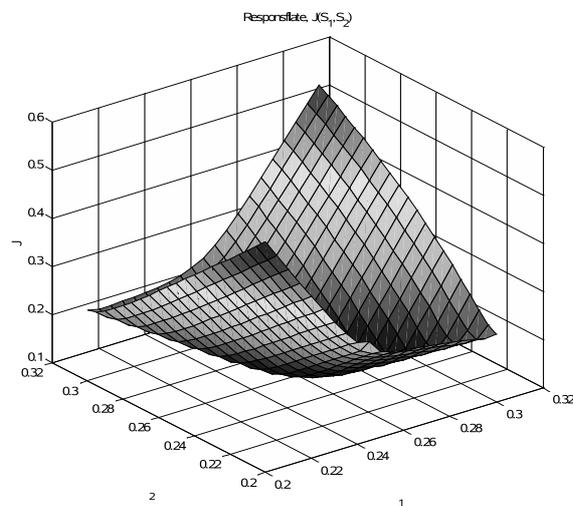


Figure 2.2: Cost function  $J$  resembles a quadratic dependency on  $S_1$  and  $S_2$ .

The liquid flow sensitivity is also considered. Here it is no longer so clear if the cost function is really quadratic, it looks like the function  $J = J(L)$  is not convex, see figure 2.4.

Next, disturbances in feed flow, concentration, boil-up and vapor split will be considered.

## 2.3 Calculation of Span

To calculate the span, an estimate of the implementation error is needed. For the temperature measurements, an accuracy of  $\pm 0.5^\circ\text{C}$  is assumed. Flow measurements are supposed to have an accuracy of  $\pm 5\%$ . This is the typical precision of commercially available flow meters of the rotameter type [Aalborg, 2005]. Relative measurement errors are for division additive [Førland, 2001]. For flow ratios, the expected implementation error is then  $\pm 10\%$ .

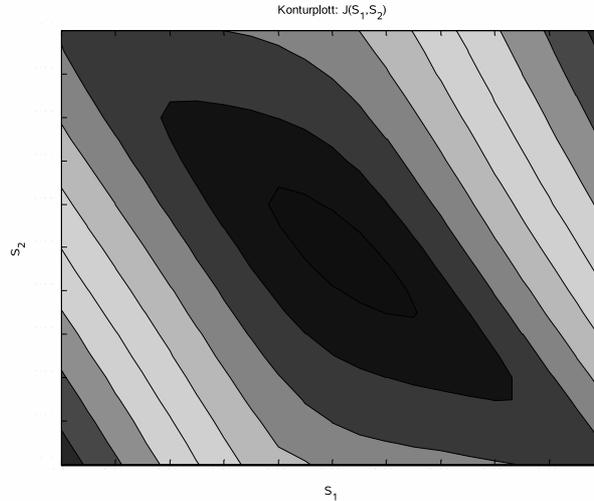


Figure 2.3: Cost function  $J$  resembles a quadratic dependency on  $S_1$  and  $S_2$ .

To calculate the span, an estimate of the optimization error is needed. This is calculated as the optimal variation:

$$\Delta e_{opt} = \frac{\max z_i - \min z_i}{2} \quad (2.2)$$

### 2.3.1 Problems in the calculation

The effect of the disturbances on  $J$  were of similar magnitude, except for the boil-up, which had a much stronger effect on the cost function. A perturbation of 1% in the other disturbances  $\{F, z_{iF}, R_V\}$  gave changes in the objective function of 1 to 12 %, whereas a perturbation in the boil-up gave a change of 70%. An optimization gave solution at  $J = 0.1631$ . This is still quite far from 0.1299, so a bracketing calculation was performed to enclose the optimum. However, bracketing with 4 degrees of freedom is a tedious task, and at last the solution was kept at  $J = 0.1365$ . For full description of the bracketing procedure, see appendix A.

## 2.4 The Scaled Gain Matrix and Optimal Selection

The model was slightly perturbed in the inputs to find the steady-state gain. The gain matrix was then scaled by the span for each variable (each row is divided by the span of the variable). The scaled gain calculation was done using Excel. This scaled gain matrix was then exported to MATLAB, using the built-in Excel link.

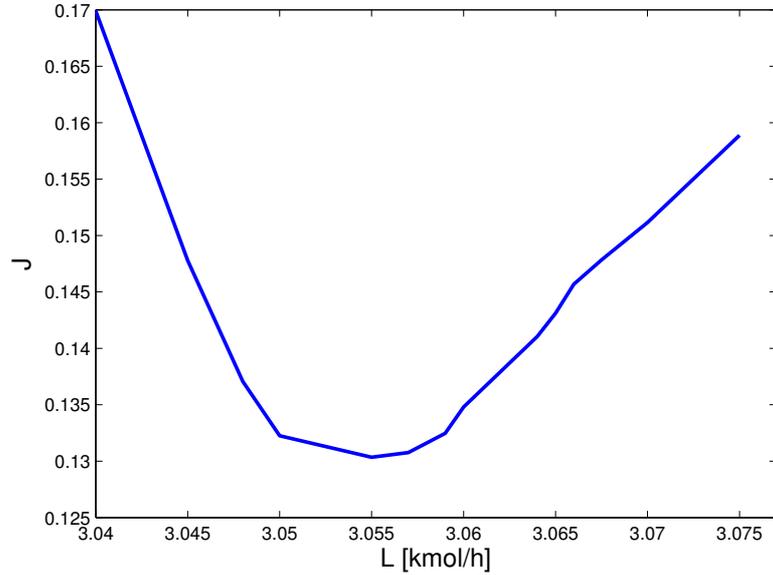


Figure 2.4: The cost function shows a non-quadratic dependence on liquid flow.

A branch and bound algorithm by Cao [Cao and Rossiter, 1997] was used to find the 3 best solutions (the 3 combinations that yield the maximum minimum singular value). This was done once with all considered variables, and once with only temperature measurements allowed. The results were as shown in Tables 2.3 and 2.4. The difference in singular values is not that big, so it might be that a selection of just temperature measurements in practice is just as good as one including internal flow ratios.

Rank	$z_1$	$z_2$	$z_3$	$z_4$	Singular Value
1	$T_5 - TS_4$	$V/B$	$T_3 - TS_2$	$T_8 - TS_1$	407.9
2	$T_5 - TS_4$	$L/D$	$T_3 - TS_2$	$T_8 - TS_1$	407.8
3	$T_5 - TS_4$	$V/B$	$T_3 - TS_2$	$T_7 - TS_1$	407.7

Table 2.3: Best selections - full variable set. TS refers to figure 2.1 on page 15.

Rank	$z_1$	$z_2$	$z_3$	$z_4$	Singular Value
1	$T_5 - TS_4$	$T_{Reboiler}$	$T_5 - TS_2$	$T_6 - TS_1$	312.8
2	$T_5 - TS_4$	$T_{Reboiler}$	$T_5 - TS_2$	$T_5 - TS_1$	312.5
3	$T_5 - TS_4$	$T_8 - TS_2$	$T_5 - TS_2$	$T_6 - TS_1$	311.7

Table 2.4: Best selections - temperatures. Also here, TS refers to figure 2.1 on page 15.

### 2.4.1 Loss Calculations

Loss calculations are performed to see if the preliminary results are promising. Some indicated measurement combinations may be infeasible, which can only be detected through a brute force calculation.

#### Full Set of Candidate Variables

A loss calculation was performed using the Hysys model. Rank 1 in 2.3 was infeasible, rank 2 was feasible but gave a negative loss for the vapor flow (boil-up,  $V$ ) disturbance ( $L = -0.006$ ). This shows that the bracketing operation had not located the real optimum. This problem may have several reasons:

- Non-convex optimization problem
- Numerical Precision problems in Hysys

It seems that the first possible reason is the one causing problems (due to non-convexity). This affects the scaling of the gain matrix, because the calculated scaling is based on an erroneous estimate of the optimal variation. However, the selection of the optimal set is probably not too sensitive to the scaling. In order to find a better estimate of the optimal variation, and a better scaling, a method for correcting the start condition of the gradient based optimization in Hysys is suggested, see section 2.5.

This method was used to recalculate the scaling for the gain matrix, and the selection was calculated again using the branch and bound method of Cao. The results are given in Table 2.5

Rank	$z_1$	$z_2$	$z_3$	$z_4$	Singular Value
1	$T_5 - TS_4$	$L/D$	$T_3 - TS_2$	$T_8 - TS_1$	406.9
2	$T_5 - TS_4$	$L/D$	$T_8 - TS_3$	$T_9 - TS_1$	406.8
3	$T_5 - TS_4$	$V/B$	$T_3 - TS_2$	$T_7 - TS_1$	406.6

Table 2.5: Best selections after scaling update - full variable set. TS refers to figure 2.1 on page 15.

The loss calculation yields that the combination with rank 3 is infeasible, and the two first combinations are both very good candidates, see Table 2.6

SVD Rank	Loss
1	0.0005
2	0.0005
3	INFEASIBLE

Table 2.6: Loss calculation - full variable set

## Temperature Subset Selection

After the discrepancy in the reoptimization at the boil-up disturbance, the temperature selection was also recalculated, but the optimal selection did not change. Hence, the selection shown in Table 2.4 is used in the calculations. However, the singular values changed slightly. The new singular values are:

- Rank 1: 312.5
- Rank 2: 312.2
- Rank 3: 311.5

These are still very similar. That is, the losses should not differ very much. However, what happens, is that no solution is found when the temperatures given in Table 2.4 are used as specifications in Hysys. This is because, these cannot be kept at constant values when other process variables are changed. The situation is probably caused because there are two temperature specifications in section  $TS_2$ , which causes the system to be overdetermined <sup>1</sup>.

It seems that the loss is not very dependent on the choice of the controlled variables, as long as the selection is feasible. This is a very attractive situation. Based on intuition, the following temperatures were selected:

- $T_5 - TS_1$ : To stabilize the temperature profile in the prefractionator.
- $T_7 - TS_2$ : Close to the reboiler, to control the purity of the bottom product.
- $T_4 - TS_3$ : Lower part of main tower: Temperature profile control.
- $T_4 - TS_5$ : Upper part of main tower: Temperature profile control

A brute force calculation with these temperatures kept at their nominal values, shows that the loss is practically zero. It seems that the important question in this case is "at what setpoints should we control the plant", and not "what should be controlled".

## 2.5 Startvalue Correction for Optimization

As explained in section 2.4.1, problems with non-convexity are often encountered. An outline of an algorithm to overcome this, is given in figure 2.5.

The fix is simply to use the best feasible solution indicated by the singular value method, using the initial scaling. Then the indicated variables are used as specifications in Hysys, and a new starting point for the reoptimization is calculated. Then the process is optimized again, and this is

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<sup>1</sup>Where Hysys gives the somewhat cryptical error message: "Singular Column Matrix: Possibly no physical solution at given conditions"

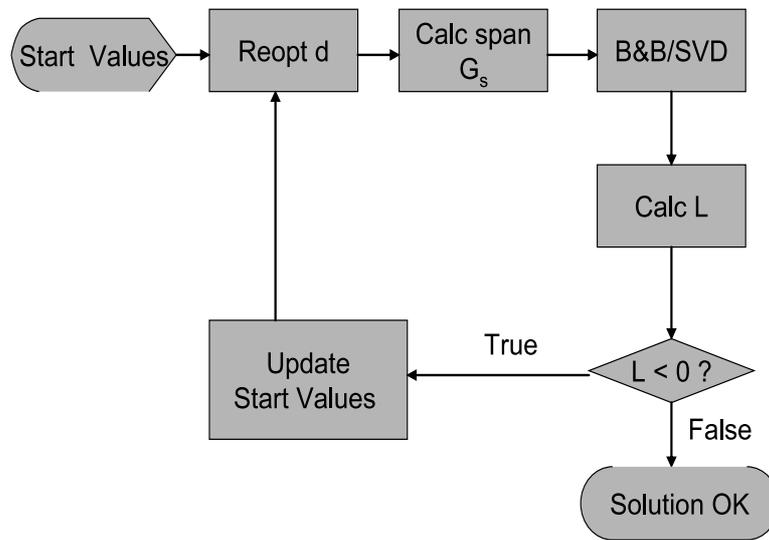


Figure 2.5: A method to overcome convexity problems

done iteratively until the loss ( $L$ ) is positive. Mostly, only one iteration is required. An illustration of what the start value correction does, is given in figure 2.6. A disturbance moves the state as shown, and a gradient based optimization method will then converge to a local minimum. A correction using the solution indicated by the singular value analysis, moves the state to a point closer to the global minimum, and the optimization then has a possibility of converging to the best solution.

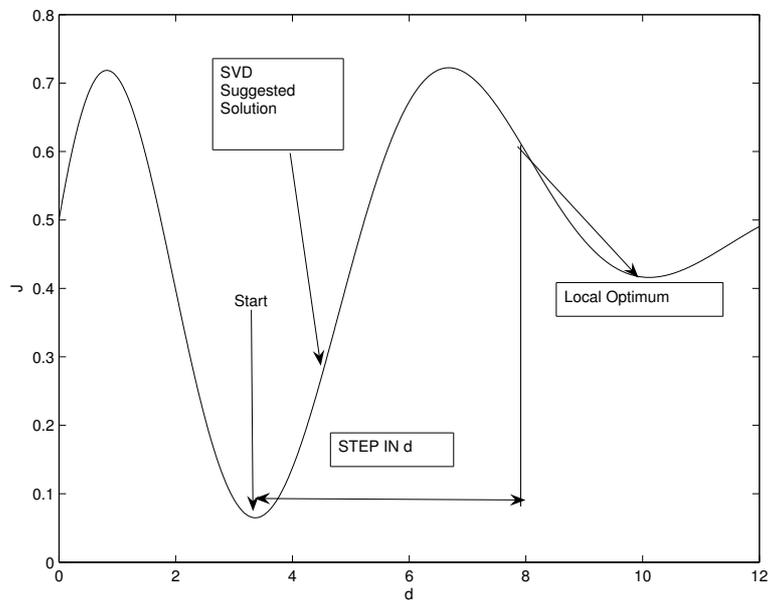


Figure 2.6: Effect of correcting the start values

## Chapter 3

# Control Configuration

An analysis of which variables to be controlled has been done. The analysis indicated that the selection of controlled variables is not critical for this application.

### 3.1 Control with Four Temperature Measurements

For the following analysis, the four temperatures indicated on page 21 are chosen as controlled variables, as shown in figure 3.1.

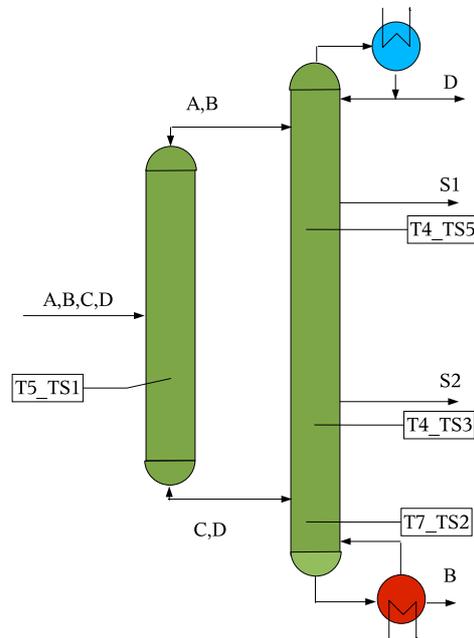


Figure 3.1: Temperature measurements in the control analysis

A dynamic simulation in Hysys was attempted to assist controller design and tuning, but the model was too unstable to be of any use. A step in any of the inputs gave large oscillations or convergence toward some solution outside the physical variable domain (negative pressures and mole fractions, for instance).

The pairing is done with regard to short loops. The prefractionator measurement  $T_5 - TS_1$  is then to be controlled using the liquid split ( $R_L$ ).  $T_4 - TS_5$  is controlled with the liquid flow (reflux,  $L$ ),  $T_4 - TS_3$  with  $S_1$  and  $T_7 - TS_2$  with  $S_2$ . The control could probably be done using PID controllers, because the measurements are not too close, such that heavy interactions are not expected. However, to determine this, dynamic simulations are necessary.

### 3.2 Sensitivity Analysis

In order to analyse the potential of the chosen outputs as good controlled variables, a sensitivity study was performed.

In the prefractionator,  $y_1 = T_5 - TS_1$  was chosen as controlled variable. Keeping all other controlled variables constant, the column purity (the cost function,  $J$ ) showed to be not very dependent on the value of  $y_1$ , which is an attractive situation. The result is given in fig 3.2 on page 27.

The top measurement in the main tower showed a much narrower minimum. This is not so attractive, and here the position of the measurement may be more important. The sensitivity analysis result is given in 3.3.

The lower measurement in the main tower is problematic. The sensitivity analysis gives a picture of the non-convexity of the optimization problem used in the first part of this work, see figure 3.4. The minimum is very narrow, hence  $y_3 = T_4 - TS_3$  is a bad choice for a controlled variable.

Regarding  $y$ , see 3.5, the minimum is even narrower. The allowable range of  $y_4$  narrower than the precision in a temperature measurement, hence the use of this variable will probably lead to controllability problems.

It seems that it is not a good idea, to try to control the lower temperatures in the column. The prefractionator temperature is ok.

The singular value method indicated that 3 temperatures and a flow ratio should be controlled. This might be a better solution.

### 3.3 Results from the Singular Value Rule

The singular value rule gave the following suggestion for the controlled variables:

- $z_1 = T_5 - TS_4$
- $z_2 = V/B$
- $z_3 = T_3 - TS_2$
- $z_4 = T_8 - TS_1$

These outputs may be better to use for control, than using just temperatures, because one avoids measurements very close to the reboiler. That is, one avoids temperature measurement, where the allowable variation is smaller than the measurement accuracy. The pairing would be done such that short loops are achieved. Some interaction between the controlled variables is to be expected. To see if self-optimizing control can be achieved, dynamic simulations must be done. If self-optimizing control can not be achieved, it might be worth considering multivariable control from the layer above, using the set-points in the regulatory layer as degrees of freedom.

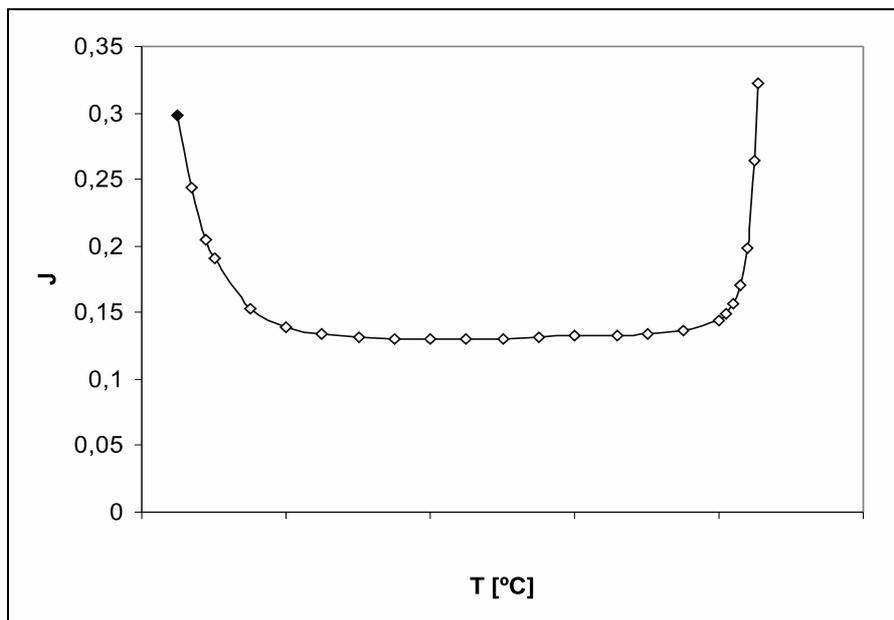


Figure 3.2: Purity,  $J$ , as a function of prefractionator temperature specification,  $y_1 = T_5 - TS_1$

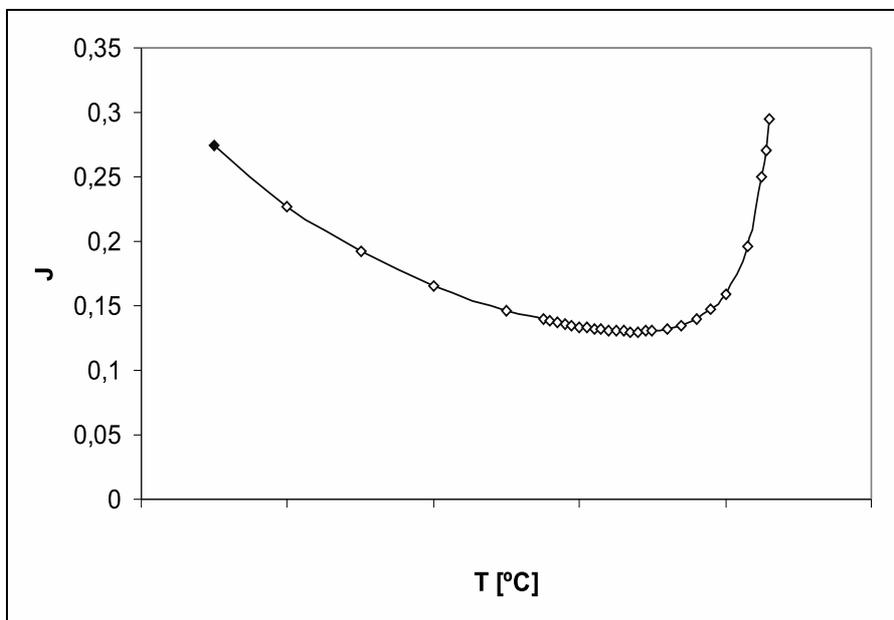


Figure 3.3: Purity,  $J$ , as a function of temperature specification,  $y_2 = T_4 - TS_5$

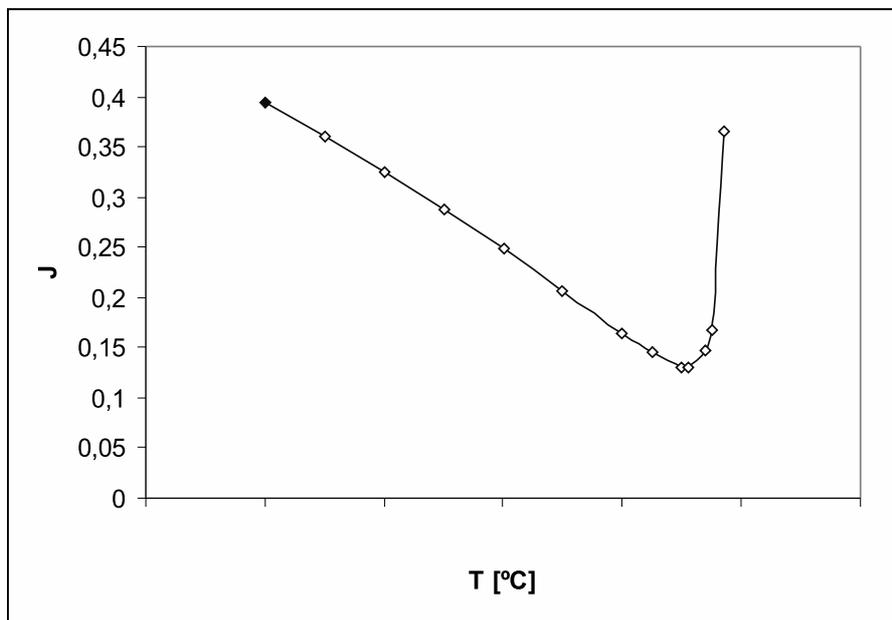


Figure 3.4: Purity,  $J$ , as a function of temperature specification,  $y_3 = T_4 - TS_3$ . A very narrow minimum.

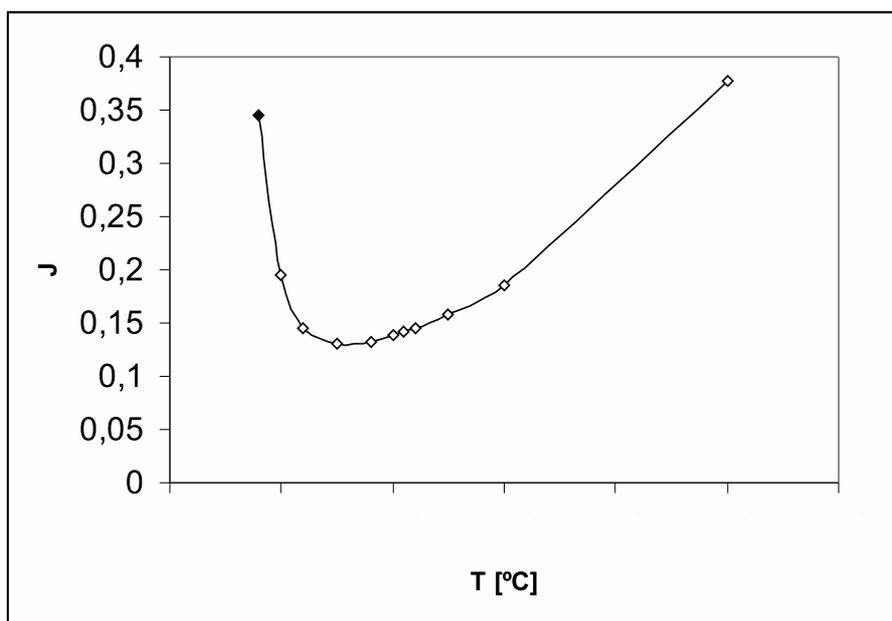


Figure 3.5: Purity,  $J$ , as a function of temperature specification,  $y_4 = T_7 - TS_2$ . A very narrow minimum.

## Chapter 4

# Concluding Remarks

In this report, it is shown that Hysys can be used for steady-state analysis of custom processes. It is, however, also found that Hysys is not good for dynamic simulation, at least, the model used for steady-state analysis can not be used.

The singular value rule is applied to the Kaibel column control structure problem, and from a steady-state point of view a good solution has been found. The indicated best solution, surprisingly, includes other measurements than just stage temperatures.

Some measures to handle non-convexity and problems with convergence are also introduced, using the singular value rule to correct the star values for optimization, using a reduced gradient method in the optimizer. The success of this method, requires that the steady-state gain of the process model is obtained close to the optimum also of the disturbed process. This requires that the global optimum does not move very much when the process is disturbed.

## Appendix A

# Bracketing Calculations

For the calculation of the optimal inputs when a disturbance in the boil-up occurs, a bracketing procedure was used. This is simply varying the inputs to locate where the optimum might be. For a non-convex multivariable problem this is a very tedious task, and hence it is mostly used in 1-dimensional optimization, as pre-optimization for gradient based methods. The calculations for the boil-up are summarized in Table A.1.

Test No.	$S_1$	$S_2$	$L$	$R_L$	$J$
1	0.22	0.22	NC	NC	0.3340
2	0.24	0.24	NC	NC	0.1794
3	0.26	0.26	NC	NC	0.3157
..	...	...	...	...	...
..	0.2442	0.2490	3.07	0.2699	0.1365

Table A.1: Bracketing Calculations

The bracketing is meant to close in the optimum, so that the optimizer can be given limits on the search region.

## Appendix B

# Software Descriptions

In the calculations, software from different vendors has been used. A short description of each program will be given, and a description of connecting calculations will follow.

### Excel

Microsoft Excel 2003 is used to calculate the gain matrix, the span and for visualizing sensitivity calculations.

### Hysys

Hysys v3.2. is a process flowsheet simulator, which is used to simulate the Kaibel distillation process at steady-state. The program includes an optimization tool, which is used to perform local optimization.

### MATLAB

MATLAB version 7.1 from MathWorks was used for branch and bound selection calculations and plotting of sensitivity graphics.

### Automation and Software Connectivity

The sensitivity studies were automated using macros written in Visual Basic for Applications (VBA) in Excel. The Hysys object library is available to Visual Basic through an extensive application programming interface (API) and can be imported into the VBA object library.

Data exchange between MATLAB and Excel is also easy to implement, thanks to the Excel link package in MATLAB 7.1. Data can be read from and written to Excel Worksheets using simple MATLAB functions.

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