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Master Thesis

**Control structure design for two
distillation columns in sequence**

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Abstract

Even for simple distillation systems with only two columns, the control problem can be significant. This project provides an initial outline of a systematic procedure for finding the optimal control structure, through identification of active constraint regions and self-optimizing variables.

The procedure is used to study a system of two distillation columns in sequence in order to find the optimal control structure. To achieve optimal control, the active constraints have to be identified and controlled tightly. Which constraints that are active depend on the external conditions. This project has mapped how the active constraints change following variations in the steam price and feed flow.

Two of the active constraint regions were studied further. A rigorous steady state analysis was conducted to find variables, which when controlled to constant value, keep the operation close to optimal. Variables with such properties are said to be self-optimizing. Controlled variables consisting of single measurements and measurement combinations have been investigated. In a constraint region with low energy price, controlling a tray temperature in the top part of the second column was found to be optimal. In a second region studied, where only the product specification of the valuable product is active, three tray temperatures that would keep the system close to optimum were identified.

Sammendrag

Selv for relativt små systemer, for eksempel et system av to destillasjonskolonner koblet i serie, kan kontrollproblemet være komplisert. Dette prosjektet skisserer en generell prosedyre for å finne den optimale kontrollstrukturen. Prosedyren prøver å finne den optimale kontrollstrukturen gjennom å identifisere aktive begrensingsregioner og selvoptimaliserende variable.

I denne hovedoppgaven har optimal kontrollstruktur av to destillasjonskolonner i serie blitt studert. For å oppnå optimal kontroll, må de aktive kontrollvariablene i systemet bli identifisert og kontrollert stramt. Hvilke kontrollvariable som er aktive, avhenger av ytre betingelser. Dette prosjektet har kartlagt hvordan de aktive variablene endres mot variasjoner i damppris og fødestrøm.

To av de aktive begrensingsregionene er studert videre. En grunding analyse ble gjennomført med systemet i stasjonær tilstand, for å finne variabler, som ved konstant verdi, vil drive systemet mot optimaltilstanden. Variabler med disse egenskapene sies å være selvoptimaliserende. Både kontrollvariabler bestående av en enkelt måling og kombinasjoner av målinger, har blitt vurdert. I begrensingsregionen med billig damp, ble det funnet optimalt å styre en trinntemperatur i den øvre delen av kolonne to. I den andre regionen som ble studert, var kun produktspesifikasjonen til det verdifulle produktet aktivt. Tre trinntemperaturer som vil holde systemet nært det optimale punktet ble identifisert.

Acknowledgments

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Declaration of compliance

I declare that this is an independent work according to the exam regulations of the Norwegian University of Science and Technology (NTNU).

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List of symbols

Symbol	Unit	Description
α		Relative volatility
Δ		Difference operator
ε		Equality constrains
$\bar{\sigma}$		Maximum singular value operator
A		Component A
B		Component B
B	<i>mol/s</i>	Bottom product flow
c		Constraint
c		Controlled variables
c^*		Nominal controlled variables
c_s		Set-point to the controlled variables
C		Component C
C°		Degrees Celsius
<i>Col.</i>		Column
d		Disturbance
d^*		Nominal disturbance
D	<i>mol/s</i>	Distillate flow
\mathbb{F}		Subscript denoting the frobenius norm
F	<i>mol/s</i>	Feed flow
G^y		Process gain matrix
G_d^y		Disturbance gain matrix
h		Step in forward and backward differences
H		Selection matrix

Symbol	Unit	Description
I		Inequality constrains
J	$\$/s$	Cost
J_{opt}	$\$/s$	Cost at optimal
L	$\$/s$	Loss
L	mol/s	Reflux flow
n		Measurement error
n_c		Number of constraints
$n_{d.o.f}$		Degrees of freedom
M		Matrix used in calculation of loss
p_F	$\$/mol$	Price feed
p_A	$\$/mol$	Price distillate column 1
p_B	$\$/mol$	Price bottom product column 1
p_C	$\$/mol$	Price distillate column 2
p_V	$\$/mol$	Price steam
q_F	mol fraction	Liquid fraction feed
T	$^{\circ}C$	Temperature
$T_{b,A}$	$^{\circ}C$	Boiling temperature pure component A
$T_{b,B}$	$^{\circ}C$	Boiling temperature pure component B
$T_{b,C}$	$^{\circ}C$	Boiling temperature pure component C
TC		Temperature controller
u		Input variables to the system
V	mol/s	Vapor flow
V_{max}	mol/s	Maximum vapor flow
W_d		Diagonal matrix giving the expected magnitude of each disturbance
W_n		Diagonal matrix with the expected magnitude of noise for each measurement
x	mol fraction	Concentration in liquid phase
x		State of the system
x_A	mol fraction	Constraint variable component A distillate col. 1
$x_{A,min}$	mol fraction	Product specification component A distillate col. 1
x_B	mol fraction	Constraint variable B distillate col. 2
$x_{B,min}$	mol fraction	Product specification component B distillate col. 2

Symbol	Unit	Description
x_C	mol fraction	Constraint component C bottom product col. 2
$x_{C,min}$	mol fraction	Product specification component C bottom col. 2
y		Output variables (measured variables)
y	mol fraction	Concentration in vapor phase
Y		Matrix used in the "exact local method"
z_F		Feed composition vector

Chapter 1

Introduction

Distillation is one of the most frequently used separation techniques in chemical industry [1]. In many cases distillation is a highly energy demanding process, and low energy consumption depends on optimal operation. Optimizing a distillation column deals with the state of the process that best fit a given set of criteria for optimal operation. When the system is exposed to a disturbance, the state of the system changes. How the system responds, depends on the control structure of the system. If the system drifts far from the optimal point, re-optimization is needed. The objective of this thesis is to identify a control structure that keeps the system close to the optimal point when exposed to disturbances, without the need to re-optimize.

The control structure of a system is highly important for optimal plant operation. A control structure problem deals with selecting the appropriate controlled variables and pairing them with variables that can be manipulated. Numerous studies have been done in this field, but few have approached the problem in a systematic fashion. The plantwide control procedure by Skogestad [2] gives a mathematical framework to the problem, and a mathematical approach is necessary in order to

identify the optimal structure in every case. Based on the mathematical framework one searches for the controlled variables that drive the system to the new optimal state when the system is exposed to disturbances. The loss is calculated by minimizing the change of a cost function. This approach to control design is well described by Larson and Skogestad [2].

1.1 Aim of the thesis

To separate three components, two distillation columns are needed. The optimal control of two distillation columns in sequence with the use of self-optimizing control, was discussed by Magnus Jacobsen as part of his PhD thesis [3]. In the present project the work of Jacobsen has been used as a basis for further studying the optimal control of two distillation column in sequence.

The aim of this thesis has been to formulate the outline of a procedure to find the primary controlled variables, and use this to study control for a system of two distillations column in sequence. Key questions are, i) how to identify active constraint regions and ii) how to find self-optimizing controlled variables. The first task was to identify a map of how the set of active constraints change as a function of feed flow and steam price. Two of the constraint regions were studied further in order to find variables that when kept constant, maintain the system close to the optimal point. In addition to study controlled variables based on single measurements, the benefit of using multiple measurement has been considered.

Chapter 2

Theoretical background

This chapter presents the theoretical background for work done in this thesis. Optimization problems are first defined mathematically, followed by a brief introduction to distillation. The principles behind active constraints, self-optimizing control and plant-wide control are explained. Methods for finding self-optimizing variables, including the "exact local method", are described towards the end.

2.1 Optimization

The problem of finding the optimal operation of a chemical plant can be structured mathematically as a constraint optimization problem. The aim is to minimize the cost function, J , within the boundaries of the system. From a practical point of view, the constraints can be product specifications, safety standards or physical limitations. This is mathematically expressed as:

$$\begin{aligned}
& \min_{x,u} && J(x,u,d) \\
& \text{subject to} && c_i(x,u,d) \leq 0, \quad i \in I \\
& && c_i(x,u,d) = 0, \quad i \in \varepsilon
\end{aligned} \tag{2.1.1}$$

Where J denotes the cost function and c denotes the constraints. Usually, the set of equality constraints includes the process model while the set of inequality constraints includes the operational constraints.

2.2 Distillation theory

Distillation is a common separation technique in chemical industry. The method utilizes the fact that for a liquid-vapor mixture at equilibrium, the lightest of two components has a higher concentration in the vapor than in the liquid. Each separation event of vapor and liquid approaching equilibrium, is called a flash. Distillation can be described as a counter-current multistage flash. From each tray in the column the vapor flows to the tray above, while the liquid flows to the tray below. By repeated separation of the vapor and liquid the mixture becomes increasingly purer. The basic principle in a distillation column is illustrated in figure 2.2.1.

The relationship between the vapor composition, y , and the liquid composition, x , is given by the equilibrium curve. The equilibrium curve in a multicomponent system with constant relative volatility, α , is given by equation 2.2.1, where i is the component number, and k refers to component with the highest boiling point [5].

$$y_i = \frac{\alpha_{ik}x_i}{1 + \sum_{j=1}^{k-1} (\alpha_{jk} - 1)x_j} \tag{2.2.1}$$

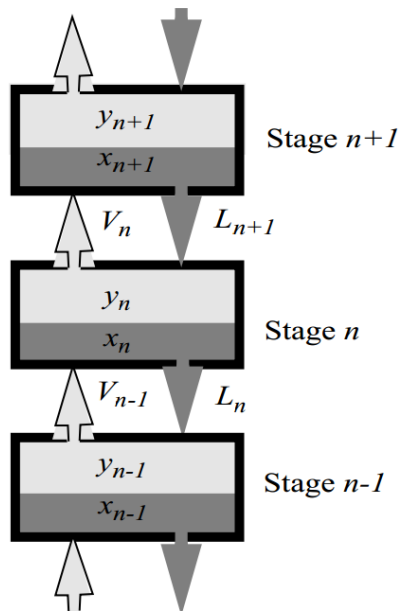


Figure 2.2.1: A distillation column modeled as a sequence of connected equilibrium stages. The light gray is the vapor phase, V , and the dark is the liquid phase, L . Where, y , denotes the composition in the vapor and, x , denotes the composition in the liquid [4].

2.3 Constraint curve and active constraint regions

A constraint is said to be active if the constraint variable in the optimal state of the system has the same value as the constraint. Identifying active constraints and finding the active constraint regions are important parts of the search for optimal plant operation. As the terms "constraint curve" and "active constraint region" are not trivial, they need to be defined. The definition is given below [3]:

Definition 1 Constraint curve:

The constraint curve corresponding to a constraint, c , is the line separating the region where c is optimally active from the region where c is optimally inactive.

Definition 2 Active constraint region:

The active constraint region is defined as the part of the disturbance space that is bounded by constraint curves, and thus have the same set of active constraints.

2.4 Plantwide control by time scale separation

The control system of a chemical plant can be hierarchically decomposed into several layers, each operating at different time scales. Typically, the layers include scheduling (weeks), site-wide optimization (days), local optimization (hours), supervisory control (minutes) and stabilizing and regulatory control (seconds) [6]. The higher layers control the layers below by providing the set-points to the subsequent layer. A sketch of a typical control hierarchy of a chemical plant is given in figure 2.4.1

When the system is exposed to disturbances, the lower layers operating on a shorter time scale would be the first to respond, trying to correct the system. The better the lower layers are to drive the system to the new optimal state, the more optimal would the whole structure be, as the system would spend less time in a non-optimal state. The core principles of self-optimizing control is to find controlled variables in the supervisory control layer, that drives the system to the new optimum when the system is exposed to disturbances, without the need for re-optimization. Variables that have these characteristics are called self-optimizing variables.

2.4.1 Self-optimizing variables

For a system to be fully specified, it is necessary to control as many variables as there are degrees of freedom. From an economic point of view it is always best to keep the system at the active constraints (for definition of active constraints

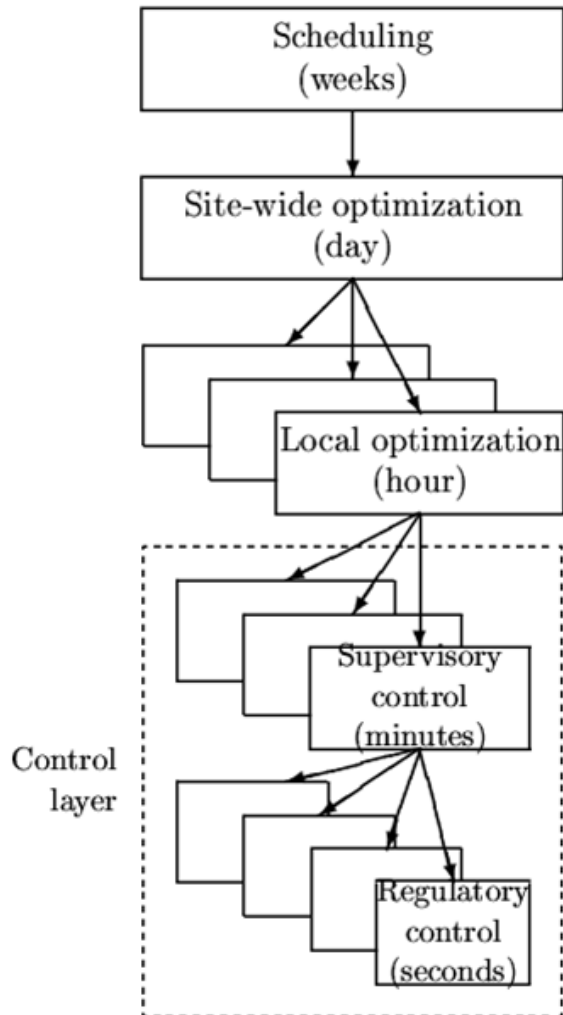


Figure 2.4.1: Typical control hierarchy of a chemical plant by time scale deviation [6].

see section 2.3). After controlling all the active constraints, the question becomes; what more to control? The preferred solution would be to find variables or combination of variables that, when held constant, maintains the systems at its most profitable state. These "magic" variables is by Skogestad et al. called

self-optimizing variables, with the following definition [6]:

"Self-optimizing control is when acceptable operation under all conditions is achieved with constant setpoints for the controlled variables."

Essentially, the task is to find controlled variables, that minimizes the loss when the system is exposed disturbances. The loss is here defined as the difference between the cost when the system is controlled and the cost at its optimal state:

$$L(u, d) = J(u, d) - J(u_{opt}, d^*) \quad (2.4.1)$$

The simplest search for self-optimizing variables is trial and error, i.e. picking a controlled variable and looking at the loss when the system is exposed to a disturbance. This method is called direct evaluation of loss. Figure 2.4.2 gives an illustration of the loss, while keeping the input, u , constant at $u = u_{opt, d^*}$, for a typical cost function.

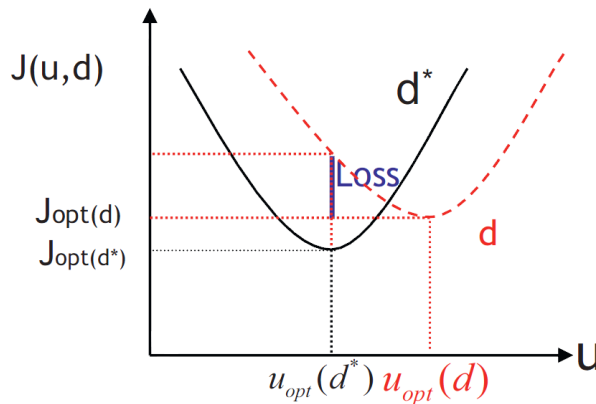


Figure 2.4.2: Illustration of loss while keeping the input, u , constant at $u = u_{opt, d^*}$ and exposing the system to a disturbance, d , [7].

The selection of controlled variables, c , from the measurements, y , can be done using a selection matrix, H :

$$c = Hy \quad (2.4.2)$$

A simplified sketch of the control problem using the selection matrix, H , is shown in figure 2.4.3.

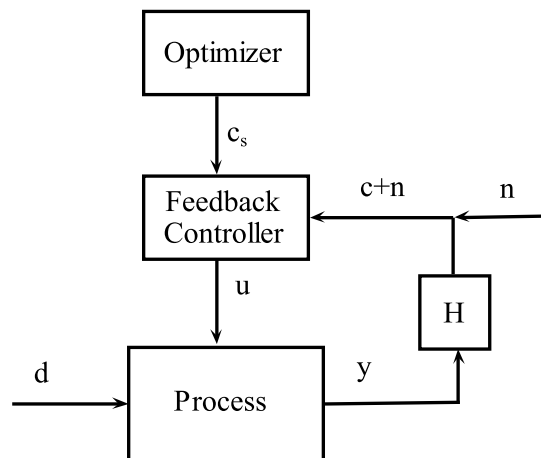


Figure 2.4.3: Control structure diagram, when selection the controlled variables, c , from the measurements, y , with a selection matrix, H . d denotes disturbances and n denotes the implementation error.

In a controlled system the input values, u , are regulated in order to keep the controlled variables, c , constant at their set-points, c_s . The magnitude of the loss depends on the controlled variables selected. Figure 2.4.4 illustrates the loss as a consequence of a disturbance, where either of the two controlled variables, c_1 , or, c_2 , are kept constant.

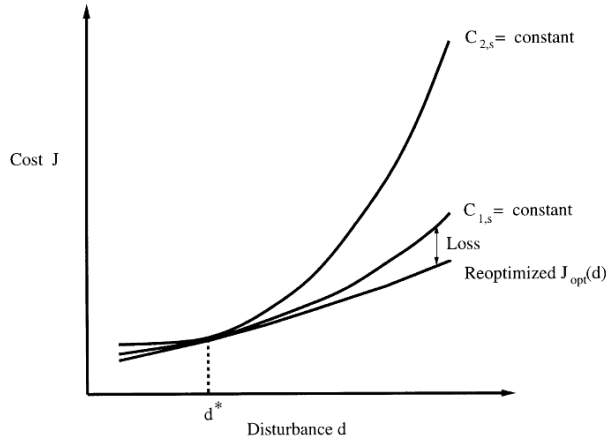


Figure 2.4.4: Illustration of loss while controlling c_1 or c_2 at there optimal values in d^* [6].

2.4.2 Exact local method

A more practical approach to search for the controlled variables is given by the "exact local method" as it includes measurements and implementation errors [8]. The objective is here to find the linear combination of measurements that would give the smallest loss. The exact local method is based on applying the following assumptions:

- Steady state cost, $J(u, d)$
- Quadratic cost approximation
- A linear model

The cost function is approximated by a Taylor expansion, neglecting higher than second order terms:

$$J(u, d) = J(u^*, d^{b*}) + [J_u^* J_d^*] \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix} + 1/2 \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix}^T \begin{bmatrix} J_{uu}^* & J_{ud}^* \\ J_{uu}^* & J_{dd}^* \end{bmatrix} \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix} \quad (2.4.3)$$

Here $\Delta u = u - u^*$ and $\Delta d = d - d^*$ are deviations from the optimum, where the optimal nominal values are marked with an asterisk. J_u and J_d are the first derivatives of the cost function. As the function is approximated around the optimal point, first order derivatives would be zero. To simplify notation further, the optimal point is shifted such that the nominal point (u^* , d^*) is zero. The same is done for the measurement, y , in the following paragraph.

A linear steady state model of the effect of the input, u , and disturbances, d , and the measurements, y , is assumed. The linear relationship becomes:

$$y = G^y u + G_d^y d \quad (2.4.4)$$

Here G^y and G_d^y are transfer functions from the input variables, u , and the disturbances, d , to the measurement, y . At steady state the transfer function is reduced to the steady state gain.

As for direct evaluation the goal of the "exact local method" is to find the selection matrix, H , that would minimize the loss. Usually, there are more than one disturbance. As the various disturbances might move the system in different directions, the magnitude of the disturbance and measurement errors, when calculating the loss, needs to be further defined. Two possibilities are considered, called "worst case" and "average loss".

- Worst case loss is the loss when the combined normalization vectors for disturbances and measurement errors have 2-norm less than 1.

$$\left\| \begin{bmatrix} d \\ n^y \end{bmatrix} \right\|_2 \leq 1 \quad (2.4.5)$$

- Average loss is the loss when the disturbance and the measurement errors

are assumed to be normal distributed.

$$\begin{bmatrix} d \\ n^y \end{bmatrix} \in N(0, 1) \quad (2.4.6)$$

Based on these definitions, expressions for the worst case and average loss can be derived. The expressions are given below as a function of H :

$$L_{wc} = \frac{1}{2} \bar{\sigma}(M)^2 \quad (2.4.7)$$

$$L_{avg} = \frac{1}{2} \|M\|_{\mathbb{F}}^2 \quad (2.4.8)$$

Where

$$M(H) = J_{uu}^{1/2} (HG^y)^{-1} HY \quad (2.4.9)$$

and

$$Y = \begin{bmatrix} FW_d & W_{n^y} \end{bmatrix} \quad (2.4.10)$$

Here $\bar{\sigma}$ denotes the maximum singular value of the matrix, M , and $\|M\|_{\mathbb{F}}$ denotes the Frobenius norm. The matrix, F , is the optimal sensitivity, defined as:

$$F = \frac{\partial y^{opt}}{\partial d} \quad (2.4.11)$$

The optimal sensitivity, F , can be obtained directly from the definition or by using equation 2.4.12.

$$F = -G^y J_{uu}^y J_{ud} + G_d^y \quad (2.4.12)$$

For a full H , meaning that there are no restrictions on the structure of H , there exists an analytical expression for H that minimizes J [7]. The expression is given in equation 2.4.13.

$$H^T = (YY^T)^{-1}G^y(G^{y^T}(YY^T)^{-1}G^y)^{-1}J_{uu}^{1/2} \quad (2.4.13)$$

2.5 Degrees of freedom

The degrees of freedom in a system is the number of variables that can vary independently [9]. A distillation column has a total of 3 degrees of freedom if the feed is fixed. Usually, pressure is controlled to a constant value, leaving 2 degrees of freedom. Connecting two distillation columns with pressure controlled, would give 2 degrees of freedom from each column, leaving the system with a total of 4 degrees of freedom.

2.6 Mathematical tools

All the coding in this thesis has been done in Matlab. The built-in solver for non-linear constraint problems "fmincon.m" was used to optimize the model. "fmincon.m" attempts to find the constraint minimum of a scalar function using an iterative solver. There are 4 possible solvers integrated in Matlab.

- trust-region-reflective
- active-set
- interior-point
- sqp

The "sqp" algorithm was found to work well, and it is used in all the optimizations in the present project. 'sqp' satisfies bounds at all iterations and has the ability to recover from infeasible results. A selection the script developed in this project is presented in Appendix C.

2.7 The "branch and bound" algorithm

The selection of controlled variables from possible measurements, using the "exact local method", has been implemented in a branch and bound algorithm by Kariwala and Cao [10]. In their work scripts developed in Matlab were used to search for optimal controlled variables by minimizing the average loss or worst case loss. The average loss calculated in the algorithm is different from the average loss using equation 2.4.8.

$$L_{avg,uniform} = \frac{1}{6(n_y + n_d)} \|M\|_{\mathbb{R}}^2 \quad (2.7.1)$$

Kariwala and Cao assumes a uniform distribution of disturbances d , and input variables, u , resulting in the following expression for average loss. Compared to the average loss in equation 2.4.8, the loss in equation 2.7.1 is scaled by a factor of $1/(3 * (n_y + n_d))$. As it is only a scaling factor separating the two equations, the optimal controlled variables would be the same for the two methods. In the present project the average loss from the "branch and bound" algorithm is scaled such that it matches the average loss in equation 2.4.8.

Chapter 3

A systematic procedure to search for the primary controlled variables

Finding good primary controlled variables is an important step in the search for optimal plant operation, and it is one of the main steps in plantwide design, as described in section 2.4. In this chapter a systematic procedure for finding the primary controlled variables in a chemical plant is outlined. The procedure is based on the plantwide control method by Skogestad [11], and attempts to find the primary controlled variables, that from a steady state point of view, would give the smallest loss.

The procedure can be divided into two main parts. The first part is to find the active constraint regions. According to Skogestad [6] it is always best to control the active constraints. The second part is to find good self-optimizing variables for the remaining degrees of freedom. Active constraint regions and self-optimizing variables are described in section 2.3 and section 2.4.1, respectively.

In the subsequent chapters, chapter 4 and chapter 5, this procedure is used to study optimal control for a system of two distillations columns in sequence.

The main steps in the procedure are illustrated in a flow diagram in figure 3.0.1.

3.1 Initial steps

There are four main initial steps that need to be carried out before the search for the active constraint regions can begin. These are:

- Define the cost function and the constraints
- Develop a mathematical model
- Identify the degrees of freedom in the system
- Identify important disturbances

The sequence of these four initial steps are irrelevant is not important.

3.1.1 Defining the cost function

The problem has to be structured mathematically as a constraint optimization problem according to equation 2.1.1. The cost function in the optimization problem measures the quality of the control structure and provides the decision criteria in the search for the optimal controlled variables. Typically, the objective is economically motivated. The optimum is thus the state that is most profitable in economic terms. Mathematically the cost, J , would be negative with respect to the profit, P ($C = -P$). Only variables that affects the steady state of the system should be included in the cost function. A typical cost function is the sum of utilities and feed, subtracted the income from the products.

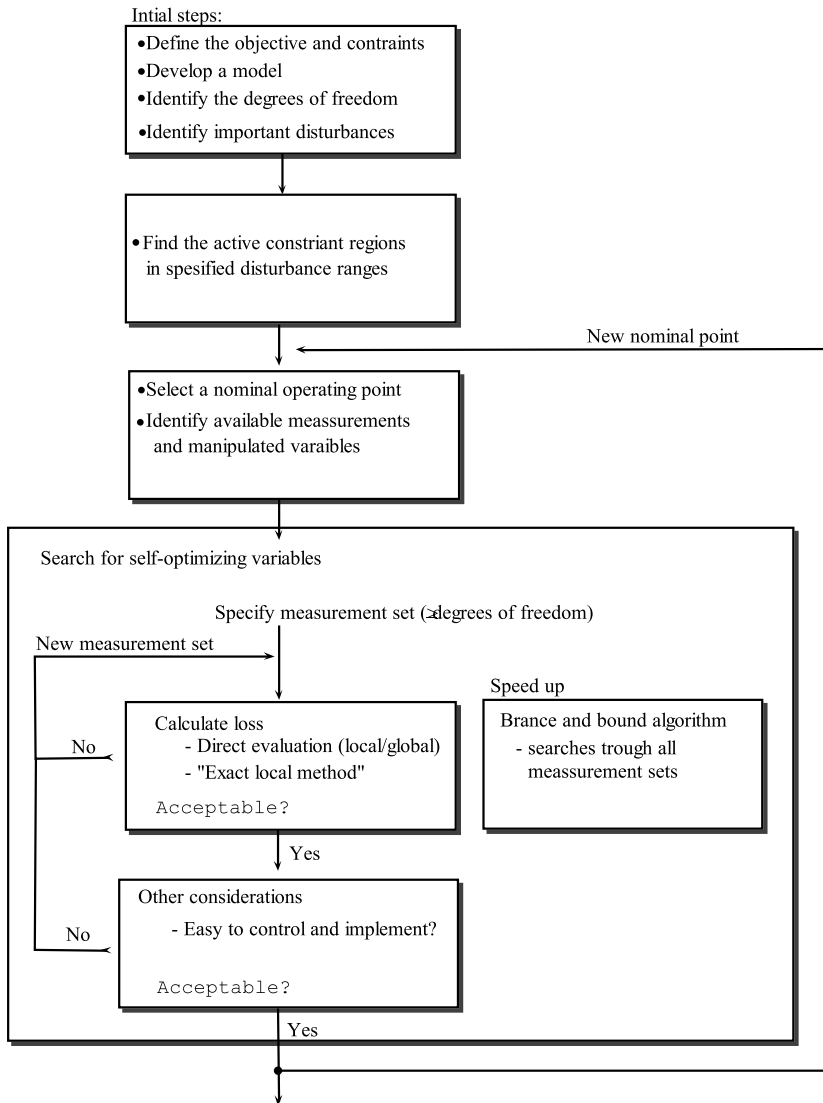


Figure 3.0.1: Main steps in a general procedure to search for the optimal primary controlled variables.

In an ideal approach the cost of the whole plant should be included. However, in

most cases this would be too complex, and the task should be divided into smaller subproblems.

3.1.2 Developing a mathematical model

Any optimization is depending on a reliable mathematical description of the system model. The search for the primary controlled variables that is outlined in this procedure assumes a steady state model of the system. The "exact local method" would in addition require the model to be linearized around the nominal point studied.

3.1.3 Identifying the degrees of freedom

The degrees of freedom are the number of variables that can be specified or controlled independently. For the system to be fully defined, the number of primary controlled variables has to be equal to the number of degrees of freedom.

3.1.4 Identifying important disturbances

Disturbances are uncontrolled variables that effect the state of the system. The control structure should be developed such that the system is kept at optimum when exposed to disturbances. Usually the disturbances are associated to the feed into the system, but also changes in active constraints should be handled as disturbances. When searching for the primary controlled variables, all disturbances that affect the cost function should be considered.

3.2 Finding the active constraint regions

In order to control the process at optimum, the active constraints have to be identified and controlled tightly at the constraint value. To achieve this it is necessary to know when the active constraints change, such that the control structure can be adjusted to the new constraint region. A map of how the active constraint regions change should be found. For a full understanding of the system, the active constraint regions would have to be explored for all possible disturbances. Each different disturbance would add another dimension to the active constraint region map.

3.3 Searching for self-optimizing variables

When the active constraint regions have been found, the system should be studied to identify additional controlled variables that would keep the state of the system close to optimum. In general, each point in the disturbance space should be studied individually. A point in the disturbance space studied is here referred to as a nominal point.

The goal of this part is to find the set of controlled variables that gives the least loss when exposed to disturbances. The simplest approach is to iterate through all available sets of controlled variables. The user would specify a set of controlled variables and evaluate the loss when the system is exposed to disturbances. Each controlled variable consists of either a single measurement or a combination of measurements at there optimum value in the normal point.

There are several possible methods to evaluated loss [12]. The loss could for instance be evaluated using "local direct evaluation", "global direct evaluation" or the "exact local method". While the global direct evaluation need a rigorous model, the "local direct evaluation" can be applied to either a rigorous model or

a linearized model. For the "exact local method" on the other hand, a linearized model is a prerequisite. Figure 3.3.1 shows the various methods to calculate loss when a set of controlled variables are specified.

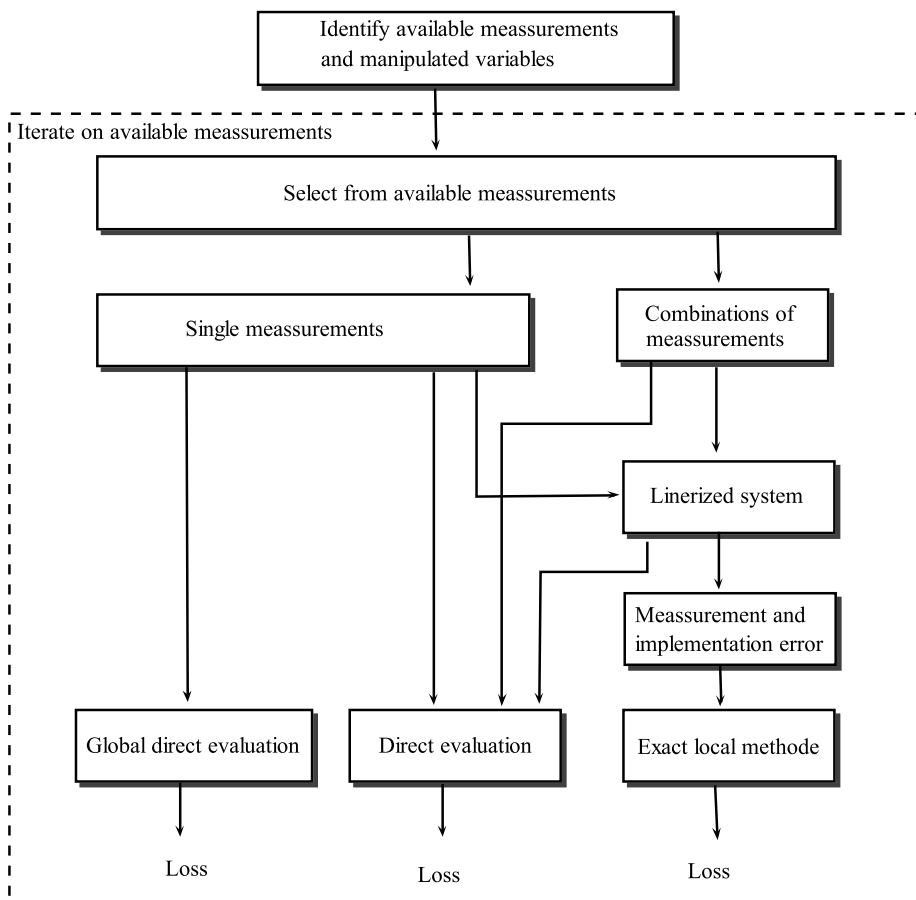


Figure 3.3.1: Methods to calculate loss when controlling a set of variables and exposing the system to disturbances. The controlled variables are selected from available measurements, either single measurement or a combination of measurements.

Even in small systems the number of possible controlled variables could be very large. This is especially pronounced if measurement combinations are used. To

reduce the number of evaluations, engineering insight could be used.

If the model is linearized, each evaluation of loss would use very little computational power. This would enable the user to search through a large number of possible controlled variables in a short time. Kariwala and Cao [10] have shown that the computational time could be further reduced using a "branch and bound" algorithm. The algorithm speeds up the process by reducing the number of evaluations needed to find the controlled variable that results in the smallest loss when exposed to disturbances.

3.4 Other considerations

The selection of controlled variables should not be based on minimization of loss alone [6]. The controlled variables should in addition be easy to measure and control accurately. A process that is difficult to control would spend longer time away from set-point, and maybe even be unstable. An offset from the set-point usually imply a loss. Keeping the process at the set-point is a prerequisite for the evaluation of loss analysis.

In cases with more than one controlled variable should the selected variables not be closely related [6], i.e. not control two tray temperatures next to each other in a distillation column. Indirectly would this requirement usually imply that the controlled variables are spread out in the process. Spreading the controlled variables may have positive effects as avoiding drift, and stabilizing all part of the process.

Chapter 4

Active constraint regions for a system of two distillation columns in sequence

A system of two distillation columns in sequence was studied, with reference to the PhD thesis of Jackobsen [3]. In order to identify the optimal control structure, the active constraint regions were mapped, and the map was subsequently compared with the one found by Jacobsen [3]. Optimal control structure in two of the regions was explored further in order to find self-optimizing variables, see chapter 5.

4.1 Model

The system studied consists of two distillation columns in sequence, separating three components A, B and C, where A is the most and C the least volatile component. The column model is based on a steady-state version of the Column A

model [13]. Both columns have 41 trays (stages) with feed entering at tray 21. The relative volatility, α , is assumed to be constant. The column uses a total condenser, meaning that all the vapor leaving the top tray is condensed. The bottom flow from column 1 is used as feed for the second column. A sketch of the model is shown in figure 4.1.1.

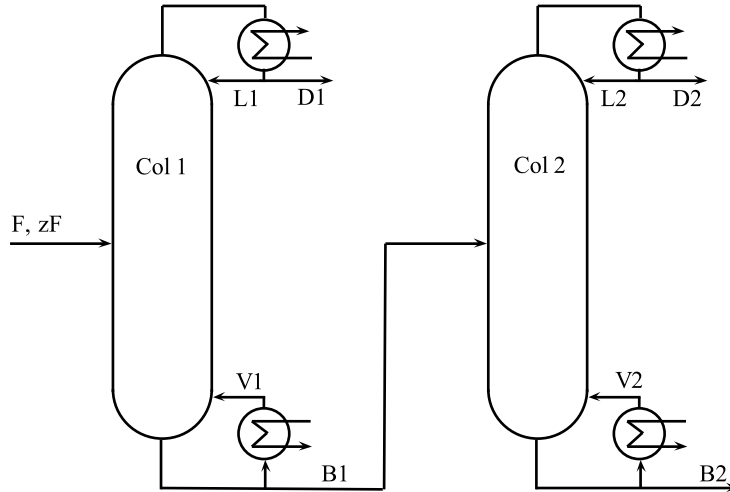


Figure 4.1.1: Illustration of two distillation columns in sequence.

4.1.1 Tray temperature estimation

The boiling temperature of a mixture is a function of the composition [4]. The temperature on each tray is estimated using the function:

$$T = T_{b,A} - (T_{b,A} - T_{b,B})x_B - (T_{b,A} - T_{b,C})x_C \quad (4.1.1)$$

Where $T_{b,A}$, $T_{b,B}$, $T_{b,C}$ are the boiling points of the pure components. Their values are given in table 4.1.1

Table 4.1.1: Boiling point of the pure components in the modeled system.

$T_{b,A}$	$100^{\circ}C$
$T_{b,B}$	$70^{\circ}C$
$T_{b,C}$	$30^{\circ}C$

4.2 The optimization problem

The system is studied to find how the optimal operation varies with disturbance. The optimal point is defined by the state of the system that minimizes the cost function within the constraints. The cost function in this case comprises the sum of the feed, the re-boiled power and the condenser power, subtracted the income from the three product flows. The condenser power is assumed to be cost free. It is also assumed that the vapor flows are restricted by a maximum value, as a real column has a finite diameter. The respective concentrations of the three product flows are being restricted to a minimum purity of 95%. A mathematical description of the optimization problem is given in equation 4.2.1.

$$\begin{aligned}
 \min_u \quad & J(u, d) = p_F F + p_V (V_1 + V_2) - p_A D_1 - p_B D_2 - p_C B_2 \\
 \text{subject to} \quad & x_A \geq x_{A,min} \\
 & x_B \geq x_{B,min} \\
 & x_C \geq x_{C,min} \\
 & V_1 \leq V_{1,max} \\
 & V_2 \leq V_{2,max}
 \end{aligned} \tag{4.2.1}$$

The system has a total of 4 degrees of freedom when feed is regarded as a disturbance. With 4 independent system variables specified, all other variables are given by the chemical properties, the component mass balances and the energy

balances.

The parameter values used in the optimization are presented in table 4.2.1. The values are the same as those used by Jacobsen [3].

Table 4.2.1: Parameter values

Parameters	Values	Units
F	Variable	mol/s
α_{AC}	2	
α_{BC}	1.5	
z_F	$[0.4 \ 0.2 \ 0.4]^T$	molfrac.
q_F	1	
p_F	1	$$/mol$
p_V	Variable	$$/mol$
p_A	1	$$/mol$
p_B	2	$$/mol$
p_C	1	$$/mol$
Constraints		
$x_{A,min}$	0.95	molfrac.
$x_{B,min}$	0.95	molfrac.
$x_{C,min}$	0.95	molfrac.
$V_{1,max}$	4.008	mol/s
$V_{1,max}$	2.405	mol/s

4.2.1 Possible number of active constraint regions

An active constraint region is defined as an area in the disturbance space which has the same combination of active constraints, see section 2.3.

According to Jacobsen [3] the maximum number of active constraint regions are 2^{n_c} . Where n_c is the number of constraints. All possible combinations are presented in Table 4.2.2. In a real system, not all active constraint regions exist.

If the constraints are independent, the number of active constraints could never exceed the degrees of freedom. As the system has 4 degrees of freedom, a constraint region where all 5 constraints are active would never occur (number 32 in table 4.2.2). In addition, the product specification of the valuable product is nearly always active. The valuable product in this case is the distillate from column 2, having the specification $x_{B,min}$. With this in mind, there are $32-16-1=15$ possible active constraint regions left. This means that there are 15 regions that are both feasible and have x_b active.

Generally, if the number of independent constraints, n_c , is smaller or equal to the degrees of freedom, the number of possible constraint regions would be limited by the number of constraints. In this case the number of possible active constraint regions would be 2^{n_c} . On the other hand, if the number of constraints are larger than the degrees of freedom, the degrees of freedom would be limiting. The number of possible constraint regions would then be reduced by the number of combinations that have more active constraints than there are degrees of freedom. A general expression for possible number of active constraint regions is presented in equation 4.2.2. The equation requires the constraint lines not to cross each other more than ones. Without this requirement the number of possible active constraint regions would be unlimited.

$$n_{regions} = \begin{cases} 2^{n_c} & \text{if } n_c \leq n_{d.o.f.} \\ 2^{n_c} - \sum_{i=n_{d.o.f.}+1}^{n_c} \binom{n_c}{i} & \text{if } n_c > n_{d.o.f.} \end{cases} \quad (4.2.2)$$

In equation 4.2.2, $\binom{n_c}{i}$ denotes the binomial coefficient.

4.2.2 Active constraint regions in the disturbance space

The system is studied to identify how the set of active constraints changes as a function of the feed, F , and steam price, p_V , at optimum. The constraint region

Table 4.2.2: All combinations of active constraints

Number	V_1	V_2	X_A	X_B	X_C	Region name
1						
2					X_C	
3				X_B		I
4				X_B	X_C	
5			X_A			
6			X_A		X_C	
7			X_A	X_B		II
8			X_A	X_B	X_C	IV
9		V_2				
10		V_2			X_C	
11		V_2		X_B		
12		V_2		X_B	X_C	
13		V_2	X_A			
14		V_2	X_A		X_C	
15		V_2	X_A	X_B		
16		V_2	X_A	X_B	X_C	
17	V_1					
18	V_1				X_C	
19	V_1			X_B		III
20	V_1			X_B	X_C	
21	V_1		X_A			
22	V_1		X_A		X_C	
23	V_1		X_A	X_B		V
24	V_1		X_A	X_B	X_C	VII
25	V_1	V_2				
26	V_1	V_2			X_C	
27	V_1	V_2		X_B		VI
28	V_1	V_2		X_B	X_C	
29	V_1	V_2	X_A			
30	V_1	V_2	X_A		X_C	
31	V_1	V_2	X_A	X_B		VIII
32	V_1	V_2	X_A	X_B	X_C	Infeasible

map is found by systematically changing the feed and the steam price and optimizing the system at each point. A grid of 150 points in each direction is used. The constraint region map is presented in figure 4.2.1.

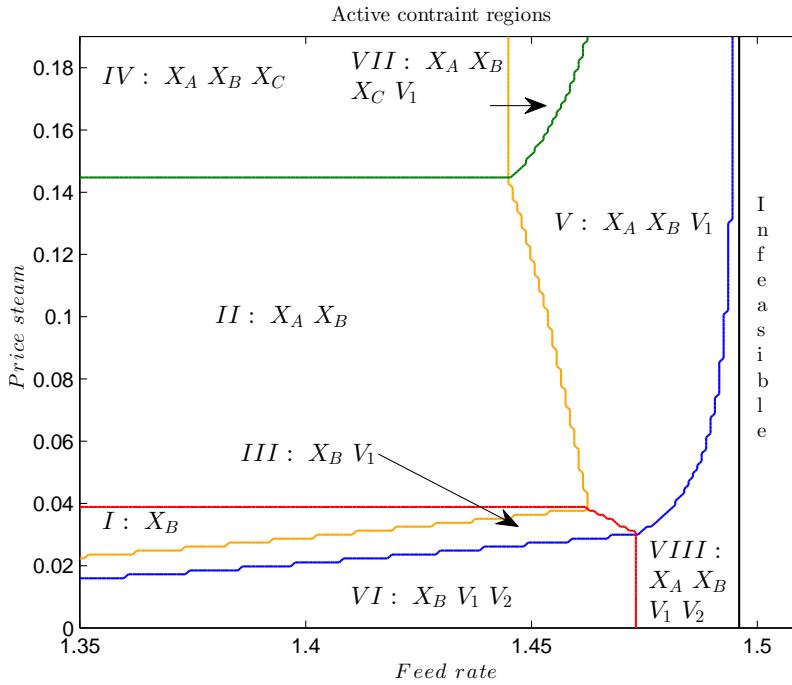


Figure 4.2.1: Active constraint regions map of two columns in sequence. The colored lines mark the border between the case when the constraint is optimally active or optimally inactive, respectively.

Numerical values for one optimization in each region are given in table 4.2.3. Most values are in accordance with Jacobsen [3]. In region VI, however, there is a discrepancy for the simulation value of $X_{A,D1}$ and $X_{B,D1}$, respectively, when the feed is set to 1.4 mol/s and the steam price is set to $0.01 \text{ \$/s}$. Their values are written in red text.

Table 4.2.3: Optimal values for selected data

Region	I	II	III	IV	V	VI	VII	VIII	IX
Column 1									
F	1.350	1.400	1.400	1.400	1.470	1.400	1.450	1.480	1.400
pV	0.030	0.100	0.025	0.025	0.100	0.010	0.180	0.010	0.160
V_1	3.853	3.870	4.008	4.008	4.008	4.008	4.008	4.008	3.892
L_1	3.300	3.290	3.436	3.436	3.400	3.437	3.408	3.396	3.312
D_1	0.553	0.580	0.572	0.572	0.608	0.571	0.601	0.612	0.580
B_1	0.797	0.820	0.828	0.828	0.862	0.829	0.850	0.868	0.820
$X_{A,D1}$	0.960	0.950	0.961	0.961	0.950	<i>0.962</i>	0.950	0.950	0.950
$X_{B,D1}$	0.041	0.050	0.039	0.039	0.050	<i>0.038</i>	0.050	0.050	0.050
$X_{C,D1}$	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
$X_{A,B1}$	0.012	0.011	0.012	0.012	0.012	0.013	0.011	0.013	0.011
$X_{B,B1}$	0.311	0.306	0.311	0.311	0.306	0.312	0.306	0.306	0.306
$X_{C,B1}$	0.678	0.683	0.677	0.677	0.682	0.676	0.683	0.682	0.683
Column 2									
V_2	2.205	2.015	2.345	2.345	2.218	2.405	2.006	2.405	1.911
L_2	1.952	1.771	2.081	2.081	1.959	2.140	1.764	2.137	1.678
D_2	0.253	0.243	0.264	0.264	0.258	0.265	0.242	0.268	0.233
B_2	0.544	0.577	0.564	0.564	0.604	0.563	0.608	0.600	0.587
$X_{A,D2}$	0.038	0.038	0.038	0.038	0.041	0.039	0.039	0.041	0.038
$X_{B,D2}$	0.950	0.950	0.950	0.950	0.950	0.950	0.950	0.950	0.950
$X_{C,D2}$	0.013	0.012	0.012	0.012	0.009	0.011	0.011	0.009	0.012
$X_{A,B2}$	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
$X_{B,B2}$	0.014	0.035	0.012	0.012	0.030	0.011	0.050	0.018	0.050
$X_{C,B2}$	0.986	0.965	0.988	0.988	0.970	0.989	0.950	0.982	0.950
J [\$/\$s]	-0.071	0.345	-0.105	-0.105	0.364	-0.201	0.841	-0.204	0.695

4.3 Discussion of the constraint region map

The constraint region map was found by optimizing the system in a grid over the whole disturbance space. This approach to mapping the active constraint regions requires substantial computational power, and is correspondingly time consuming. However, the time needed, is substantially reduced if one uses the solution in one point as initial guess for the neighboring point. This procedure will also increase the robustness and ensure that the algorithm would find a solution for every feasible point. Even with this procedure, however, the computational time would be long.

The computer used approximately six hours to calculate the active constraint map in figure 4.2.1. The calculation was conducted on a Dell, Latitude E6400 with Windows 7, Intel[®] Core[™]2 Duo P9500 processor (2.53GHz). The number of points evaluated when creating the map was $150 \cdot 150 = 22500$. This give an average of approximately 1 second per evaluation. For large systems it is expected that each evaluation would take substantially more time. If the active constraint region should be mapped in 3 disturbance dimensions, the number of evaluations needed with a grid of 150 would be $150^3 = 3.4 \cdot 10^6$, translating into a computational time of approximately $6 \text{ heures} \cdot 150 = 37.5 \text{ days}$. With this extensive time consumption this method is probable impractical, calling for the development of smarter algorithms that would reduce the time for each evaluation and the number of evaluations needed. The use of faster computer languages might of course also be considered.

Chapter 5

Case study: Self optimizing variables in region I and VI

In each active constraint region there is a unique set of constraints which are active at optimum [3] . To keep the system at optimum, all the active constraints have to be controlled tightly. Two columns in sequence have a total of 4 degrees of freedom (assuming that the pressure is controlled to a constant value and thus not included). When the active constraints are controlled, the degrees of freedom are reduced by the number of active constraints. In this chapter, region I and VI are studied to find what further variables to control, using the remaining degrees of freedom, in order to keep the process operation close to optimal.

According to Skogestad [6], the controlled variables should have the following characteristics:

- Their optimal value should be insensitive to disturbances.
- They should be easy to measure and control.
- Their value should be sensitive to changes in the manipulated variable.

- For cases with two or more controlled variables, the selected variables should not be closely correlated.

The goal is to find variables, that when kept constant, maintain the system at its optimum state when exposed to disturbances.

5.1 Potential variables to control

In this modeled system there are over a hundred potential variables which might be controlled, either as single variable or as a combination of variables. These include:

- 41 tray temperatures and compositions
- 8 flows: $D_1, B_1, V_1, L_1, D_2, B_2, V_2, L_2$

The variable to be controlled has to be connected with one of the variables amenable to manipulation, which in this case are the flow variables only:

- 7 flows: $D_1, V_1, L_1, D_2, B_2, V_2, L_2$

In this project only *LV* column structure is considered. *LV* structure denotes the case where the flows L and V , are used to manipulate the primary controlled variables. Causing the level in the reflux drum and the re-boiler drum to be controlled by the flows D and B , respectively. The primary controlled variables denote the controlled variables that eliminate the steady-state degrees of freedom.

5.2 Disturbances considered

All uncontrolled variables should be considered as disturbances. In this system, the feed is the only uncontrolled variable effecting the system, thus assumed to be the source of the dominating disturbances. Examples include changes in

feed flow, feed concentration and liquid vapor fraction. Variations in a tightly controlled active constraint could also be regarded as a disturbance. To reduce the complexity of the optimization problem, only three disturbances have been considered:

Table 5.2.1: Disturbances considered

Disturbance
Feed flow
Feed composition: zF_A at the expence of zF_B
Feed composition: zF_B at the expence of zF_C

5.3 Case 1: Selection of controlled variables in constraint region VI

In region VI, both vapor constraints V_1 and V_2 are active. In addition the concentration constraint on the valuable product x_b is active. The system has 4 degrees of freedom. As 3 of these are active, and therefore being controlled, there are 1 degree of freedom left. The region is first studied in order to find the boundaries to infeasibility. This calculation is done to better understand the behavior of the region. Assessment of the region boundaries is followed by a direct evaluation of the loss, focusing on the variables in table 5.2.1. Finally, the system was linearized and studied further using the "exact local method".

5.3.1 The boundaries of the region with respect to the reflux L_1

When V_1 , V_2 and X_B are controlled to there constraint values, there is only 1 degree of freedom left. The value of this last degree of freedom has to be such that it is possible to keep the system within the boundaries of the allowed values of

the two non-active constraints. Within the set of possibly manipulated variables, only L_1 and D_1 are realistic choices to eliminate the last degree of freedom. From the mass balance it follows that $V+(1-q)F=D_1+L_1$. As V_1 is fixed and active and $q=1$ (liquid feed only), the change in V_1 has to be negative to the change in L_1 , hence $dL=-dV$. Thus, if the limitation of one variable is found, the other is given by the mass balance.

By increasing and decreasing the reflux L_1 it is found that the system is limited at both ends. When L_1 is reduced, the top product get less pure. If L_1 is reduced too far, however, the composition constraint on the top product of column 1 would be breached. On the other hand, if L_1 is increased too much, it would not be possible to keep the bottom product of column 2 within the product specifications: When the reflux L_1 increases, the amount of component A (the most volatile) in the bottom product increases. To satisfy the specification of the top product of column 2, the reflux of this column must increase. At one point the reflux has increase so much that is no longer possible to keep both the top and the bottom products simultaneously within the desired product specifications. In figure 5.3.1, the values of the constraint variables X_A and X_C are plotted as a function of the reflux L_1 .

Furthermore, the highest and the lowest possible reflux, L_1 , was plotted as a function of the feed flow. Here, the highest and lowest value correspond to a situation where either the constraint on x_C or x_A is active, respectively. The graph is shown in figure 5.3.2 together with the optimal reflux L_1 .

Describing how L_1 changes when a variable is controlled might give a good indication of what variables would be useful for controlling the system. The ideal variable should be such that L_1 is kept at the optimal line. The value of L_1 as a function of the feed flow when a selected tray temperature is controlled to a constant value, is presented in figure 5.3.3. Correspondingly, the value of L_1 as a function of the feed flow when L_1 , L_1/F and D_1/F , respectively, are kept constant, is presented in figure 5.3.4.

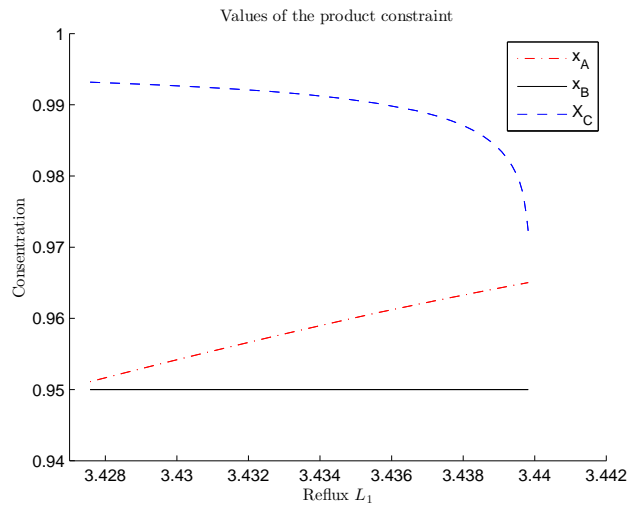


Figure 5.3.1: Values of product specifications as a function of the reflux L_1 in constraint region VI.

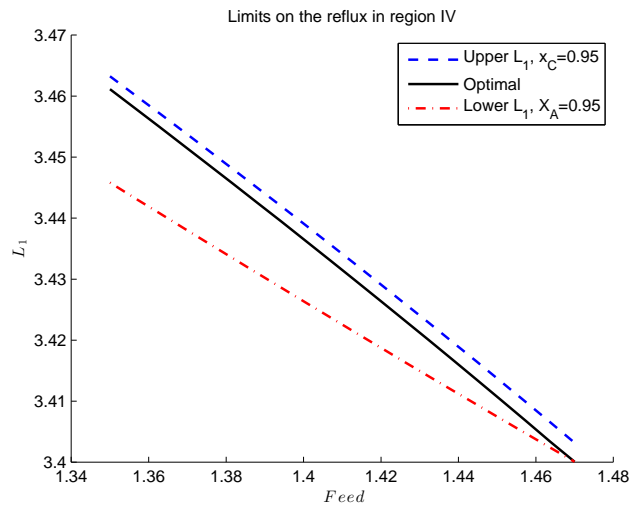


Figure 5.3.2: The highest and lowest possible values of L_1 before a constraint is breached at different feed rates.

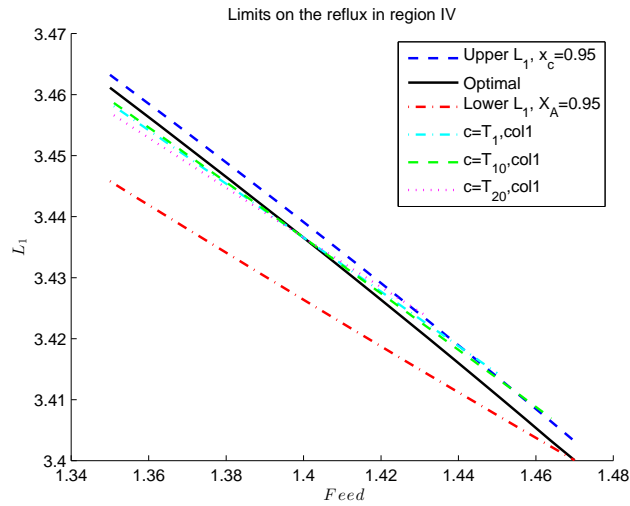


Figure 5.3.3: The value of L_1 when selected tray temperatures are kept constant.

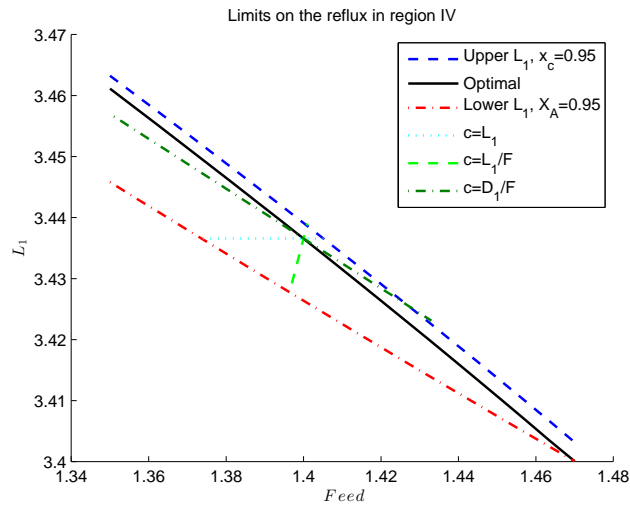


Figure 5.3.4: The value of L_1 when flow related variables are kept constant.

The value, L_1 , when controlling the temperature at tray 10, is reasonably close

to the optimal line, indicating that this would be a good controlled variable for disturbances in feed, see figure 5.3.3. Figure 5.3.4 shows that keeping, L_1 , or the ratio, L_1/F , constant, would lead to large loss and quickly move the system into the infeasible area.

5.3.2 Direct evaluation of loss

The loss when the system is exposed to a disturbance can be readily evaluated when a single variable is controlled to a constant value. Several possible candidates were held constant at their optimal values at the nominal point. The resulting loss when the system is exposed to selected disturbances is shown in table 5.3.1. The re-optimized value of the controlled variable candidates are presented in table 5.3.2.

Table 5.3.1: Table of loss for selected controlled variable candidates

Controlled variable Candidates [10^{-3} \$/s]	$F = 1.41$	$F = 1.39$	$zF =$ 0.39]	$zF =$ 0.41]	$zF =$ 0.40]	$zF =$ 0.40]	Average
Variables from column 1							
L_1	Inf	0.0850	0.2695	Inf	0.0176	0.2805	Inf
D_1	Inf	1.8425	Inf	Inf	0.1520	0.2805	Inf
$x_{A,b1}$	0.0028	0.0023	0.0148	0.0374	0.4029	0.2587	0.1198
$x_{A,d1}$	0.4422	0.2197	0.3997	0.2591	0.6611	3.2566	0.8731
$T_{bim, col1}$	0.0643	0.0453	Inf	Inf	Inf	Inf	Inf
$T_{10, col1}$	0.0378	0.0285	0.0315	0.0159	0.6059	0.3816	0.1835
$T_{20, col1}$	0.1728	0.1055	5.9639	1.0073	0.0011	0.0025	1.2088
$T_{30, col1}$	0.3004	0.1641	1.4796	0.6025	0.6636	3.3786	1.0981
$T_{top, col1}$	0.4424	0.2198	0.3992	0.2589	0.6608	3.2535	0.8724
Optimal tray from column 1	10	10	9	9	21	21	
$T_{1, opt}$	0.0378	0.0285	0.0016	0.000	0.0000	0.0002	
D_1/F	Inf	1.8425	Inf	Inf	0.1520	0.2805	Inf
L_1/F	Inf	0.0850	0.2695	Inf	0.0176	0.2805	Inf
L_1/D_1	Inf	0.5164	1.7265	Inf	0.0937	0.2805	Inf
Variables from column 2							
$T_{bim, col2}$	0.0203	0.0181	0.2124	0.1382	0.0333	0.0328	0.0758
$T_{10, col2}$	0.0127	0.0115	0.2193	0.1413	0.0797	0.0856	0.0917
$T_{20, col2}$	0.0012	0.0012	0.2297	0.1481	0.2873	0.3547	0.1704
$T_{30, col2}$	0.0000	0.0000	0.0051	0.0030	0.0213	0.0256	0.0092
$T_{top, col2}$	0.0002	0.0002	0.0577	0.0393	0.0001	0.0000	0.0162
Optimal tray from column 2	26	27	28	28	41	41	
$T_{opt, col2}$	0.0000	0.0000	0.0002	0.0000	0.0513	0.0393	0.0151

Table 5.3.2: Optimal values for the controlled variable candidates

CV candidates	Nominal	$F =$ 1.41	$F =$ 1.39	$zF =$ 0.39]	$zF =$ 0.41]	$zF =$ 0.40]	$zF =$ 0.40]
L_1	3.437	3.432	3.442	3.451	3.423	3.438	3.435
D_1	0.5714	0.5765	0.5664	0.5575	0.5854	0.5703	0.5727
$x_{A,b1}$	0.01255	0.01249	0.01261	0.01269	0.01234	0.01192	0.01318
$x_{A,d1}$	0.9618	0.9603	0.9633	0.9602	0.9633	0.9646	0.9588
$T_{btm,col1}$	89.77	89.80	89.75	89.43	90.13	90.28	89.27
$T_{10,col1}$	72.57	72.66	72.48	72.65	72.51	72.90	72.25
$T_{20,col1}$	59.96	60.09	59.82	60.44	59.49	59.97	59.94
$T_{30,col1}$	39.96	40.18	39.74	40.41	39.53	39.46	40.47
$T_{top,col1}$	31.53	31.59	31.47	31.59	31.47	31.42	31.65
D_1/F	0.4082	0.4089	0.4075	0.3982	0.4182	0.4074	0.4090
L_1/F	2.455	2.434	2.476	2.465	2.445	2.456	2.454
L_1/D_1	6.014	5.952	6.076	6.189	5.846	6.028	5.999
$T_{btm,col2}$	99.68	99.67	99.69	99.64	99.71	99.69	99.66
$T_{10,col2}$	97.23	97.16	97.30	96.95	97.49	97.41	97.04
$T_{20,col2}$	90.71	90.68	90.74	90.32	91.10	91.22	90.19
$T_{30,col2}$	77.78	77.79	77.77	77.91	77.67	78.08	77.50
$T_{top,col2}$	68.76	68.76	68.75	68.82	68.70	68.76	68.76

The direct evaluation of loss indicates that the bottom composition of column 1, $X_{A,b1}$, or a tray temperature in the top part of column 2, would be both be good variables to control. The loss is small when exposed to the disturbances considered and the re-optimized value remains close to the nominal value.

The table of loss shows clearly that controlling any of the flows, L_1 or D_1 directly, should be avoided. This is also the case for controlling a ratio between the flows, D_1/F , L_1/F or L_1/D_1 . The loss is large and the system would quickly become infeasible. In the infeasible region there is no solution to the system that would satisfy all constrains.

5.3.3 Global direct evaluation of loss controlling a tray in column 1

Distillation is not a linear process, thus the loss when a system is exposed to a disturbance would not vary linearly. To better understand the behavior of the modeled system in this project, the loss when exposed to disturbances in feed flow or feed concentration was calculated over a wide span of the disturbance.

The loss when varying the feed flow, and controlling each tray temperature individually at their nominal optimum is shown in figure 5.3.6. Correspondingly, the loss when varying feed composition (of either component A over B, or component B over C), while controlling tray temperature, is plotted in figure 5.3.7 and 5.3.6, respectively. In all cases the nominal point refers to a feed flow of 1.4 mol/s and a steam price of 0.01 $$/mol$.

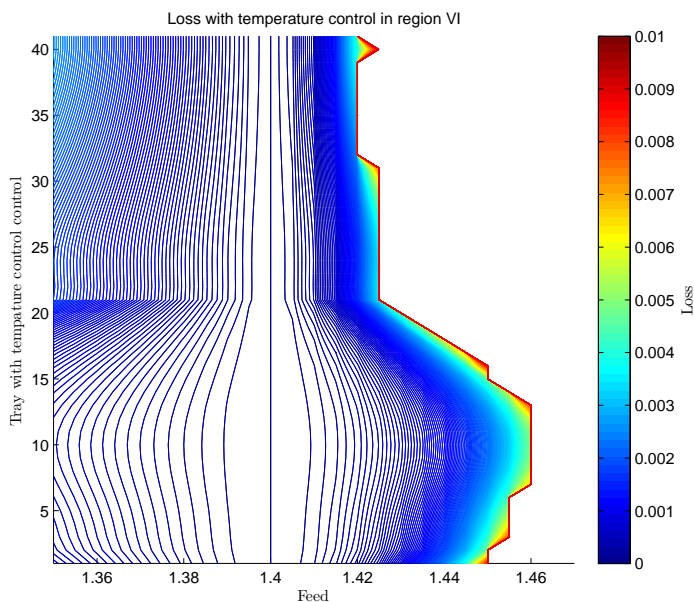


Figure 5.3.5: Loss when controlling a tray temperature and varying the feed flow to the first column. The white area outside the "red line" is infeasible $[\$/s]$.

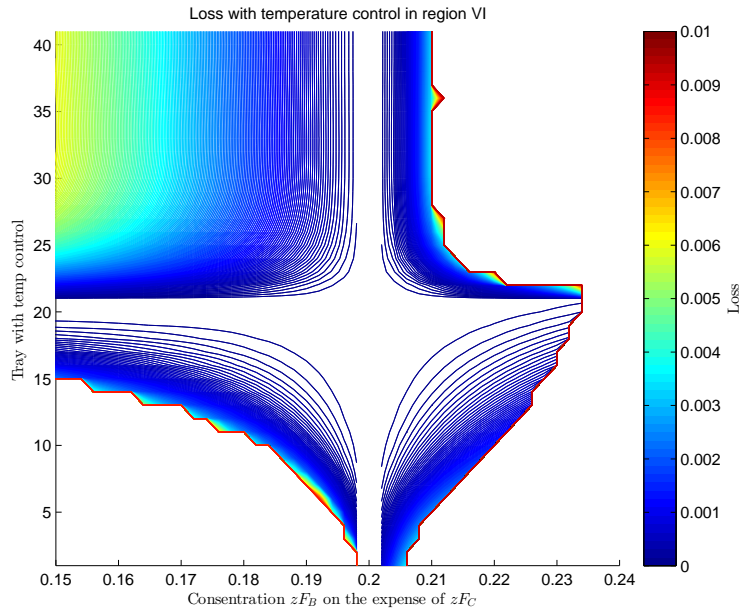


Figure 5.3.6: Loss when controlling a tray temperature and varying the feed concentration of component A at the expense of component B. The white area outside the "red line" is infeasible [\$/s].

5.3.4 Discussion of global evaluation of loss

The global direct evaluation of loss reveals that for disturbances in the feed flow it is less important which tray temperature being controlled (figure 5.3.5). Tray 10 gives the smallest loss, but its value is not significantly worse than the loss when controlling the least optimal tray temperature. To respond correctly to a disturbance in feed composition, on the other hand, the tray should be selected with care. For a disturbance in feed concentration of component A at the expense of component B, controlling the temperature around tray 9, would give close to zero loss. All other tray temperatures lead to significant loss and quickly brings the system into the infeasible region when the disturbance increases. Disturbance

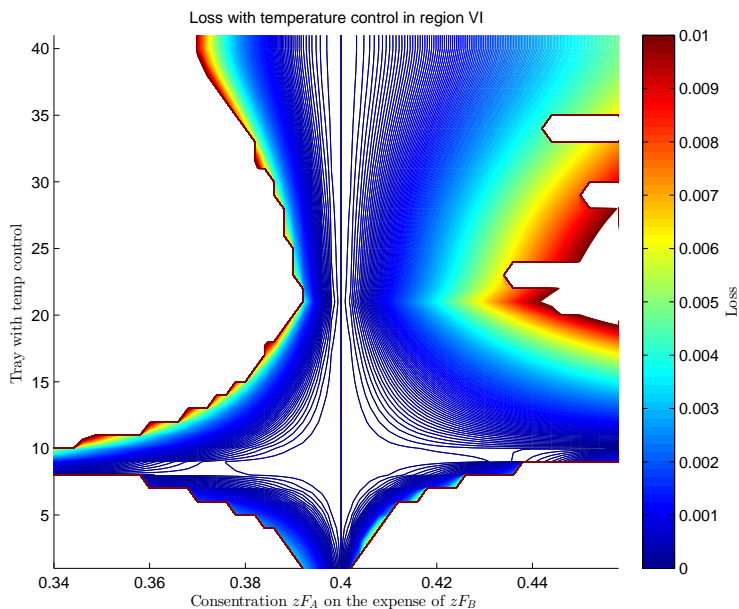


Figure 5.3.7: Loss when controlling a tray temperature and varying the feed concentration of component B at the expense of component C. The white area outside the "red line" is infeasible. The solver had convergence problems at the right side of the plot [\$/s].

in the feed concentration of component B at the expense of component C behaves similarly. To get the smallest loss in this case, the temperature of tray 20 or below should be controlled. As there are no tray that would give a small loss for these three disturbances, a combination of measurements might be necessary.

5.3.5 Global direct evaluation of loss controlling selected variables from both columns

The loss when controlling the variable candidates from table 5.3.2 was plotted over a wide range of the feed flow disturbance. This provides a more visual

picture of which controlled variables that give a small loss. The loss following disturbance in feed flow for column 1 and column 2, respectively, is plotted in figure 5.3.8 and figure 5.3.9.

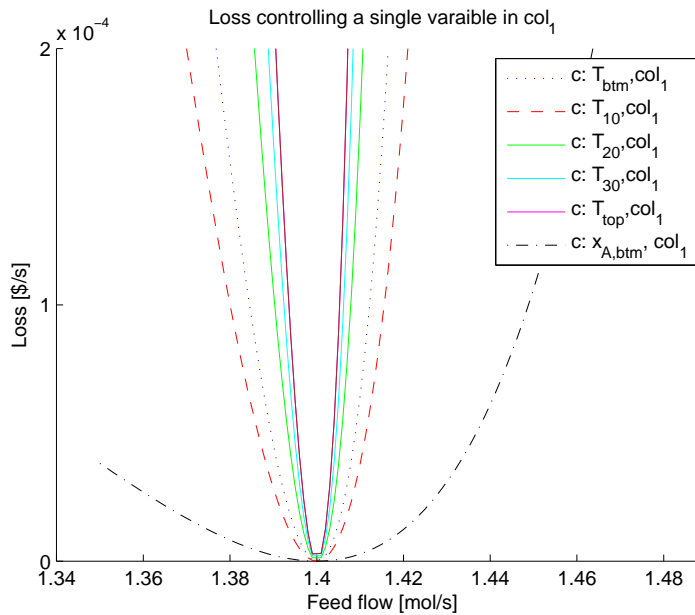


Figure 5.3.8: The loss as a function of the feed flow when controlling a variable in column 1 at its nominal optimum. The nominal feed value is 1.4 mol/s

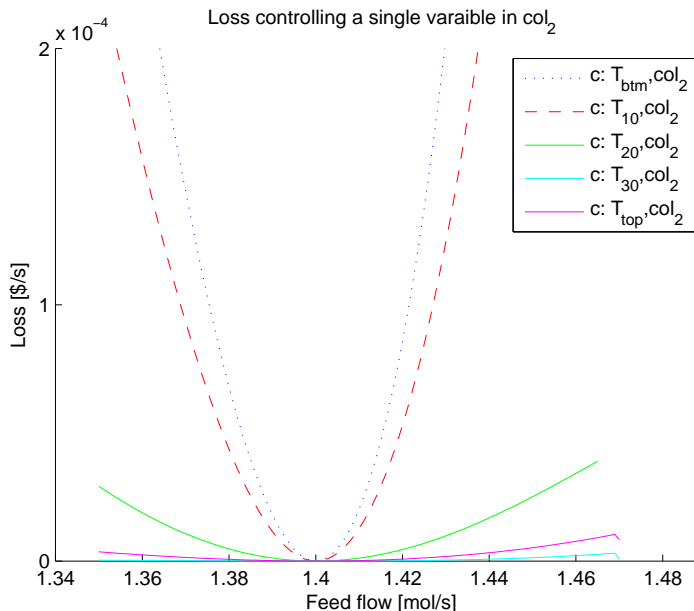


Figure 5.3.9: The loss as a function of the feed flow when controlling a variable in column 2 at its nominal optimum. The nominal feed value is 1.4 mol/s .

5.3.6 Gain and optimal sensitivity in constraint region VI

Controlling tray temperature is a common way of controlling a distillation column. According to Skogestad [1] the gain should be large and the optimal sensitivity to disturbances small. The gain and the sensitivity in constraint region VI have been calculated when the feed is at 1.4 mol/s and the steam price is $0.01 \text{ $/mol}$, using finite differences. The reflux in column 1, L_1 , was used as the manipulated variable, assessing disturbances in feed and feed composition according to table 5.2.1. The temperature process gain with respect to the input variables and the disturbances is shown in figure 5.3.10. The optimal sensitivity, F , was found for the same nominal point and is shown in figure 5.3.11.

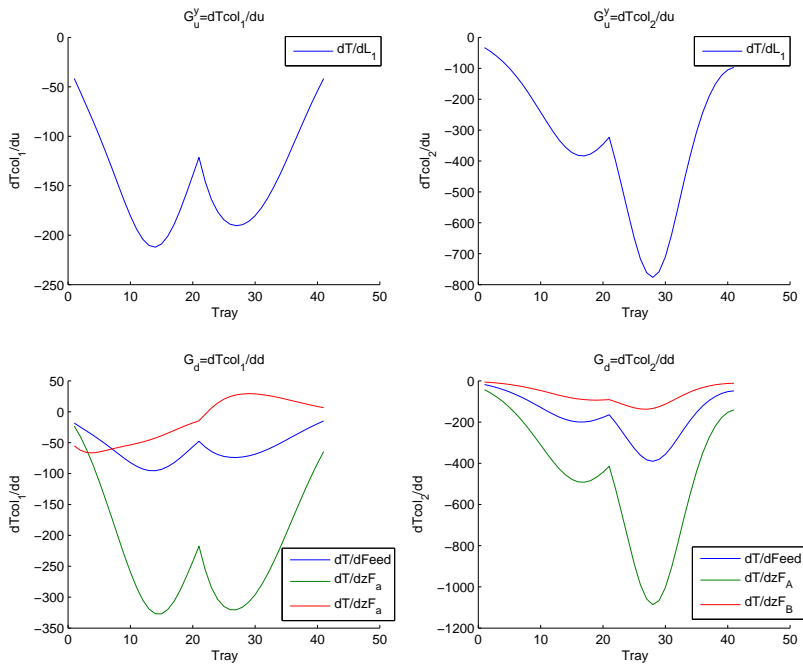


Figure 5.3.10: Process and disturbance gain in the point when feed= 1.4 mol/s and steam price= 0.01 \$/mol. The top figures show the process gain with respect to tray temperature for column 1 (left) and column 2 (right). The bottom figures show the disturbance gain with respect tray temperature in either column 1 (left) or column 2 (right).

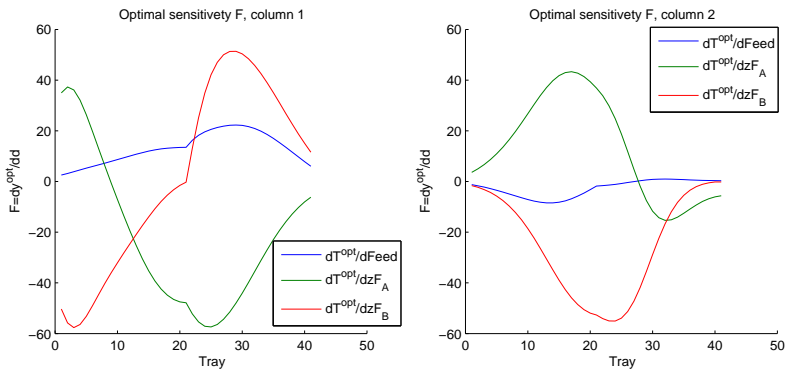


Figure 5.3.11: The optimal sensitivity in the nominal point, feed= 1.4 mol/s and steam price 0.01 \$/mol.

5.3.7 The "Exact local method" with single measurement as controlled variable

The model was linearized using finite differences (Appendix A) and the "exact local method" 2.4.2 was used to find the single tray temperature that, when exposed to disturbance, would give either the smallest average loss or worst case loss. Measurement and implementation errors have been included. To speed up the process a "branch and bound" algorithm developed by Kariwala and Cao [10], was used to search for the optimal tray temperature. The magnitude of the expected disturbance and the noise in the measured variables used in the optimization, are given in table 5.3.3.

Table 5.3.3: Magnitude of expected disturbance and noise

Expected disturbance	
Feed	0.01 mol/s
zF_A at the expense of zF_B	0.01
zF_A at the expense of zF_C	0.01
Noise in measured variable	
Tray temperature	0.5°C
Tray concentration	0.01°C

When a single controlled variable is to be selected, the matrix, M , in the definitions of worst case as well as average loss (equation 2.4.5 and 2.4.6), would be reduced to a vector. For a vector, the maximum singular value and the Frobenius norm have the same value. Thus, the worst case loss and the average loss would be the same.

The "exact local method" was used to find the single tray temperature that, when controlled, would give the minimum worst case loss. The predominating disturbances are assumed to be changes in feed flow or feed composition. Changes in the feed concentration ratio between either component A and B or B and C,

were considered. The loss from the "exact local method", when controlling a temperature in column 1 or column 2, are presented in figure 5.3.12 and 5.3.13, respectively.

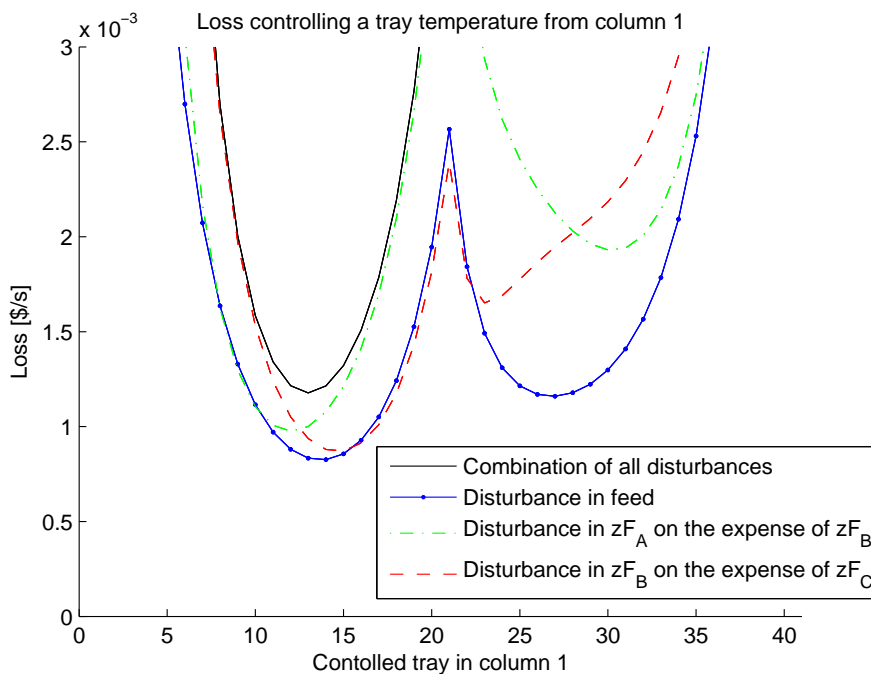


Figure 5.3.12: Loss when controlling a tray temperature in column 1, based on "exact local method".

The optimal tray temperature to control in column 1 or column 2, based on the "exact local method", are presented in table 5.3.4.

Table 5.3.4: Optimally controlled tray when calculating average- and worst case loss

Optimal loss	Controlled tray	Average-/worst case loss [\$/s]
Tray from column 1	13	$1.17 \cdot 10^{-3}$
Tray from column 2,	29	$9.35 \cdot 10^{-4}$

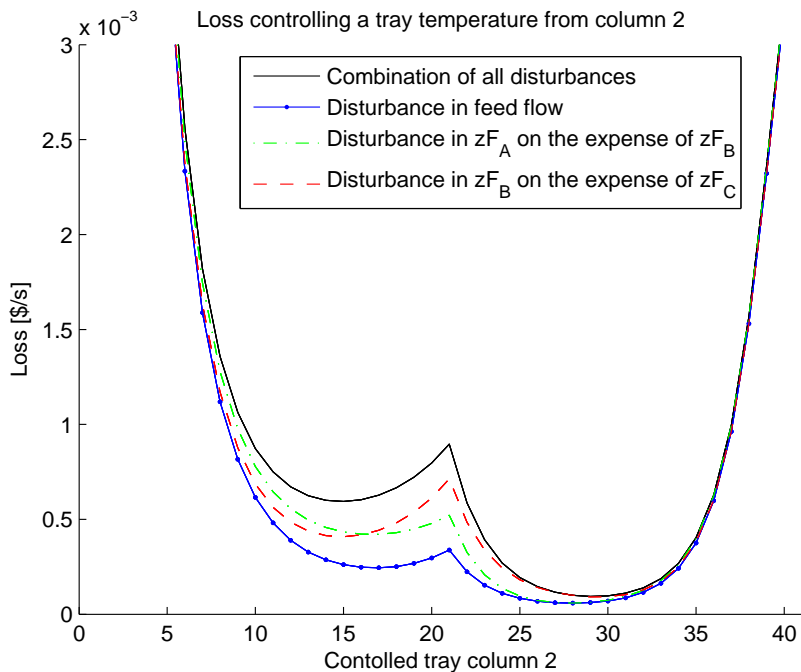


Figure 5.3.13: Loss when controlling a tray temperature in column 2, based on "exact local method".

5.3.8 Combinations of tray temperature measurements

In many cases combinations of measurements to control a variable might lead to smaller loss than using a single measurement. The "branch and bound" algorithm from Kariwala and Cao [10], was used to find the optimal combination of tray temperatures selected from either of the two columns separately. The algorithm calculates the optimal subset of measurements based on either the worst case or the average loss criteria. As only a single controlled variable is to be found, the worst case and the average loss would be the same (see section 5.3.7). Figure 5.3.14 shows the lowest possible loss when controlling a specified number of tray temperatures. The corresponding optimal tray and the respective value of

loss are presented in table 5.3.5, when only trays from column 1 are selected, and in table 5.3.5, when only trays from column 2 are selected.

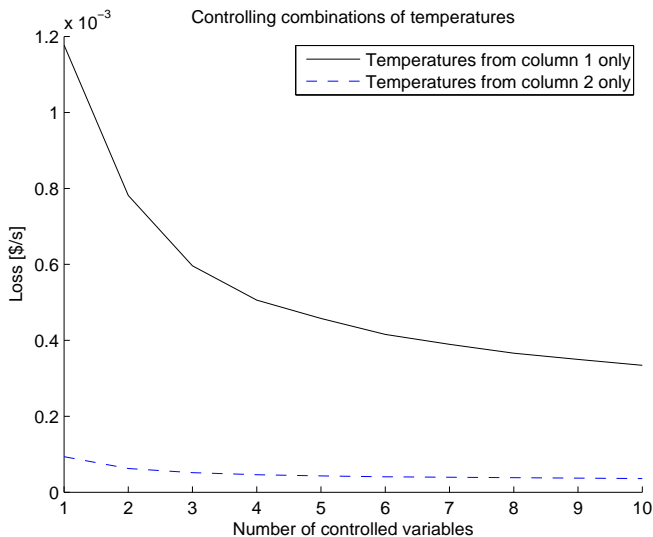


Figure 5.3.14: Lowest loss when controlling a specified numbers of tray temperatures for either column 1 or column 2, respectively.

5.3.9 Discussion measurement combinations

The "exact local method" shows that the use of combination of measurements would give a substantial reduction of loss in the case when only temperatures from the first column were selected. Controlling a combination of the three best tray temperatures would reduce the loss by approximately 50% of the loss when controlling the temperature in the single best tray. However, even with a combination of 10 measurements, using a single tray in the top part of the second column would be substantially better.

Table 5.3.5: Optimal tray combinations selected from column 1, based on exact local method

n_y	Optimal trays to control	Worst case-/ average loss [10^{-3} \$/s]
1	13	1.1775
2	12 13	0.7817
3	10 11 31	0.5964
4	10 11 12 32	0.5059
5	9 10 11 12 31	0.4577
6	8 9 10 11 31 32	0.4155
7	8 9 10 11 31 32 33	0.3894
8	7 8 9 10 11 31 32 33	0.3660
9	6 7 8 9 10 11 31 32 33	0.3498
10	6 7 8 9 10 11 31 32 33 34	0.3343

Table 5.3.6: Optimal tray combinations selected from column 2, based on exact local method

n_y	Optimal trays to control	Worst case-/ average loss [10^{-3} \$/s]
1	29	0.0938
2	29 30	0.0624
3	29 30 31	0.0515
4	29 30 31 32	0.0461
5	29 30 31 32 33	0.0432
6	28 29 30 31 32 33	0.0408
7	28 29 30 31 32 33 34	0.0394
8	10 28 29 30 31 32 33 34	0.0385
9	11 21 28 29 30 31 32 33 34	0.0372
10	10 11 21 28 29 30 31 32 33 34	0.0362

5.3.10 Direct evaluations of loss for combinations of tray temperatures

The loss was calculated when controlling the optimal combination of tray temperatures from table 5.3.5 and table 5.3.6, and exposing the system to the three

disturbances in table 5.2.1 individually. The results for either column 1 or column 2, are presented in table 5.3.7 and table 5.3.8, respectively.

Table 5.3.7: Table of loss when controlling the optimal combination of tray temperatures from table 5.3.5

n_y	$F = 1.41$	$F = 1.39$	$zF =$ 0.39]	$zF =$ 0.41]	$zF =$ 0.40]	$zF =$ 0.40]	Average [10^{-3} \$/s]
			0.21,	0.19,	0.19,	0.21,	
			0.40]	0.40]	0.41]	0.39]	
1	0.0435	0.0323	0.2770	0.1568	0.1520	0.1338	0.1326
2	0.0419	0.0312	0.2210	0.1282	0.1899	0.1600	0.1287
3	0.0813	0.0564	0.1926	0.1156	0.0308	0.0246	0.0836
4	0.0743	0.0521	0.1907	0.1146	0.0466	0.0384	0.0861
5	0.0748	0.0525	0.1683	0.1011	0.0596	0.0486	0.0842
6	0.0928	0.0634	0.1371	0.0831	0.0377	0.0277	0.0736
7	0.0882	0.0606	0.1397	0.0852	0.0440	0.0330	0.0751
8	0.1029	0.0693	0.1154	0.0700	0.0341	0.0234	0.0692
9	0.1086	0.0727	0.0976	0.0586	0.0382	0.0256	0.0669
10	0.1128	0.0751	0.0951	0.0573	0.0323	0.0207	0.0655

Table 5.3.8: Table of loss when controlling the optimal combination of tray temperatures from from table 5.3.6

n_y	$F = 1.41$	$F = 1.39$	$zF =$ 0.39]	$zF =$ 0.41]	$zF =$ 0.40]	$zF =$ 0.40]	Average [10^{-3} \$/s]
			0.21,	0.19,	0.19,	0.21,	
			0.40]	0.40]	0.41]	0.39]	
1	0.0002	0.0001	0.0194	0.0100	0.2824	0.3405	0.1088
2	0.0002	0.0002	0.0328	0.0182	0.2475	0.2977	0.0994
3	0.0003	0.0002	0.0473	0.0273	0.2192	0.2629	0.0929
4	0.0003	0.0003	0.0611	0.0361	0.1973	0.2361	0.0885
5	0.0004	0.0003	0.0730	0.0437	0.1812	0.2163	0.0858
6	0.0003	0.0003	0.0560	0.0326	0.2055	0.2456	0.0900
7	0.0004	0.0003	0.0645	0.0380	0.1930	0.2301	0.0877
8	0.0000	0.0000	0.0413	0.0248	0.2001	0.2377	0.0840
9	0.0000	0.0000	0.0557	0.0357	0.1623	0.1920	0.0743
10	0.0000	0.0000	0.0422	0.0282	0.1584	0.1866	0.0692

Table 5.3.7 and table 5.3.8 present the loss when exposing the system to the disturbances individually and controlling a tray temperature combination. This shows how much the loss is reduced, for the individual disturbances, when adding extra measurements. In addition it can be seen that a disturbance in zF_A at the expense of zF_B , is the major source of loss, when controlling a combination of temperatures from the first column. Disturbance in zF_B at the expense of zF_C is the major source of loss when controlling a combination of trays from the second column.

5.4 Case 2: Selection of controlled variables in constraint region I

In active constraint region I, only the concentration constraint of the valuable product is active. Thus, there are 3 degrees of freedom that must be controlled. The input gain, the disturbance gain and the optimal sensitivity, F , were all determined for the nominal point when feed were set to 1.35 mol/s and the steam price were $0.03 \text{ \$/mol}$. The gain is shown in figure 5.4.1 and the sensitivity in figure 5.4.2. Reflux to column 1, L_1 , and the two boil-ups, V_1 and V_2 , were chosen as manipulated variables.

5.4.1 Optimal control using single temperature measurements

The "exact local method" implemented in a "branch and bound" algorithm, described in section 2.7 was used to search for the temperature measurements that would give the least loss when exposed to a disturbance in the feed flow of 0.01 mol/s and a disturbance in the feed composition of $0.01 \text{ mol fraction}$. The measurement error for the tray temperatures was assumed to be $\pm 0.5^\circ\text{C}$. The input values were presented previously in table 5.3.3. The set of tray temperatures that in this case gives the smallest loss is presented in table 5.4.1.

Table 5.4.1: Tray numbers for optimal control of the system in region I according to average loss and worst case loss calculations

Optimal temperature control	Column 1	Column 2	Loss
Average loss	32	12, 30	$1.10 \cdot 10^{-3}$
Worst case loss	33	8, 27	$2.77 \cdot 10^{-4}$

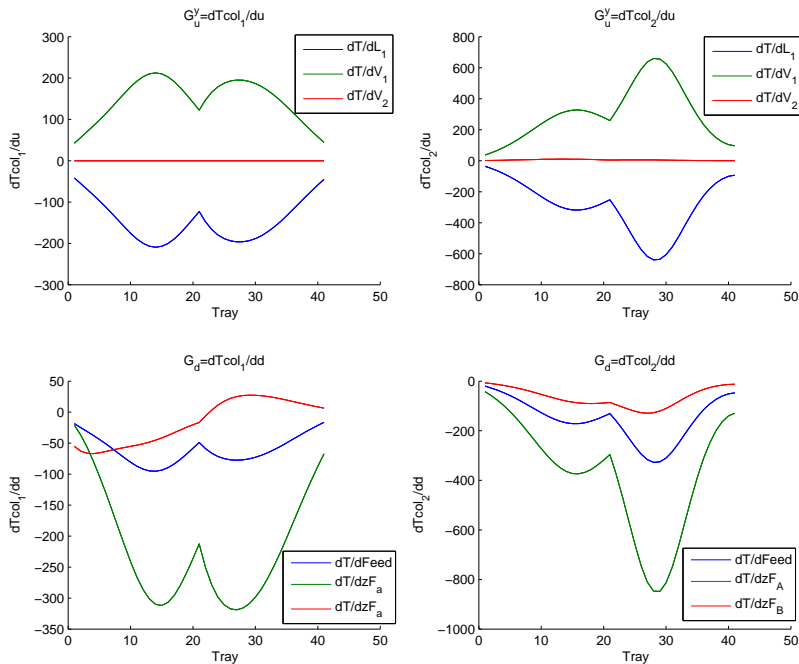


Figure 5.4.1: Process and disturbance gain in the point when feed= 1.35 mol/s and the steam price= 0.03 \$/mol. The top figures shows the process gain with respect to tray temperature for either column 1 (left) and column 2 (right). The bottom figures show the disturbance gain with respect to tray temperature in column 1 (left) and column 2 (right)

5.4.2 Discussion optimal control in constraint region I

In section I it was found to be optimal to control one tray in the top part of the first column and simultaneously two trays in the section column. The trays found were all located approximately halfway between the feed tray and the top or bottom of the column, respectively. By comparing the location of the trays in figure 5.4.1 and figure 5.4.2, the optimal tray seem to be located in areas that has a good trade-off between high gain and low optimal sensitivity. This is

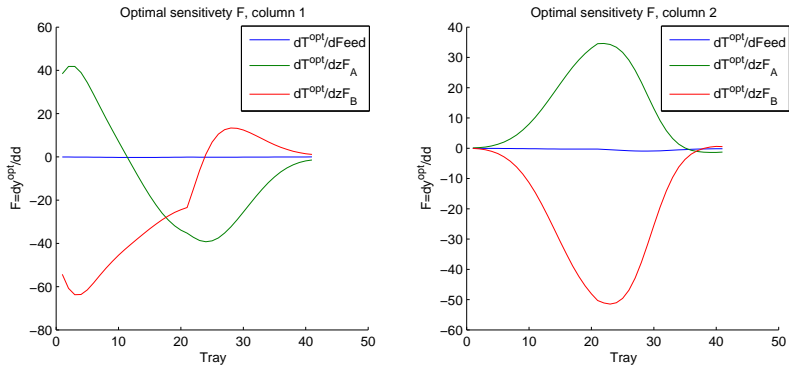


Figure 5.4.2: The optimal sensitivity with respect all temperature for either of the two columns. The three considered disturbances are i) feed flow, ii) feed composition change between component A and B and iii) feed composition change between composition B and C

accordance with Skogestad [1], suggesting that the gain of the optimal controlled variable should be high and the optimal sensitivity small.

Chapter 6

Discussion

In this section the results described chapter 3, chapter 4 and chapter 5 are explained and discussed. The discussion follows the natural progression of the work , starting with the systematic procedure used to find the primary controlled variables (chapter 3). This is followed by a discussion of the active constraint region (chapter 4) map and two case studies (5).

6.1 Systematic procedure

The systematic procedure outlined in chapter 3, presents the major steps in the process of finding the optimal control structure. It should be possible to implement the procedure in an atomized computer program. The scripts developed in this project cover the core part of such a program, although some of the scripts are case specific. The scripts are presented in appendix C. The code developed to find the active constraint region map and the code concerning the "exact local model" can handle any model, but the script used to linearize the model is unfortunately limited to the three disturbances presented in table 5.2.1.

6.2 Active constraint regions

The active constraint region map was found by optimizing the system over a grid covering the whole disturbance space. As previously stated, this is very computationally demanding. A major advantage is that it is independent of human intervention. In addition the algorithm can run the problem in parallel, thus take advantage of an increasing number of cores in modern CPU's.

Jacobsen proposed a method for finding a constraint region map but required manual considerations to reduce the number of optimization calculations. For example, he argues that if the region border (which is part of the constraint curve) is independent of one of the disturbances considered, that part of the line would be straight, and can be defined by two points only. Such assumptions reduce the number of optimization calculations, but requires substantial human intervention and is vulnerable to human error.

The active constrain region map found in the present project, figure 4.2.1, was compared to the map found by Jacobsen. The two maps are identical except for the border between region V and VII, and between II and V. Jacobsen approximates these borders with straight lines, while the analyses done in the present project has found the borders to be curved. The constraint map found by Jacobsen are presented in figure 6.2.1. The colors on the border lines refer to the different constraints.

It should be noted that the system considered in the present thesis is fairly simple. For larger systems the number of constraints and the computational time for each optimizations would be substantially higher. As previously mentioned, the grid algorithm used in this thesis would be too slow to be used in practice for more complex systems. This calls for the development of faster algorithms.

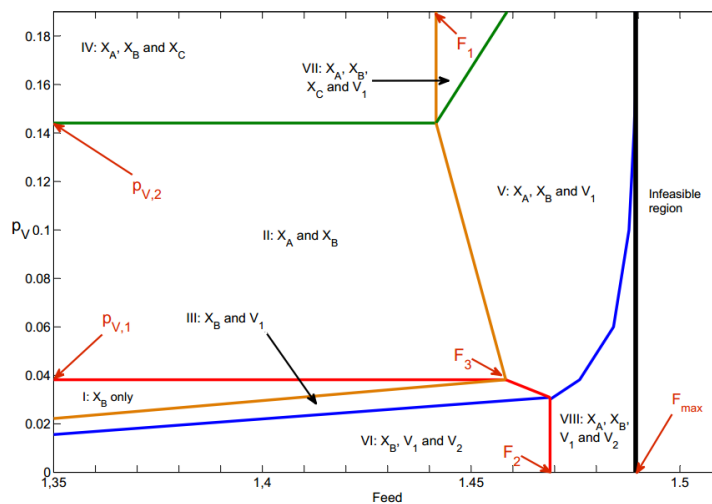


Figure 6.2.1: Active constraint region map for two columns found by Jacobsen [3]. The colors of the border lines refer to the different constraints.

6.3 Case studies

Constraint region VI was studied in detail to find good self-optimizing variables to control the remaining degrees of freedom. The two main approaches were the "direct evaluation of loss" and the "exact local method". The system was in some cases also studied over a selected segment in the disturbance space ("global direct evaluation"). All approaches indicate that the best alternative would be to control a single tray temperature in the top part of the second column. This would keep the system close to optimum and the loss would be insignificant. From figure 5.3.10 and figure 5.3.11 it can be seen that optimal sensitivity is small while the steady state gain is large. This is in accordance with Skogestad [1], stating that the optimal sensitivity should be small and that the gain from the manipulated to the controlled variables should be large.

In section VI, only reflux, L_1 , and distillate flow, D_2 , in the first column, are

in practice the only variables amenable to manipulation. The substantial physical distance between the manipulated variables and the location of the possible controlled variable would make the response slow and control difficult. Thus, if a tray in the top of the second column should be used a direct coupling would make the control slow and hard to use in practice. However, this problem could be overcome using a cascade. Figure 6.3.1 show a outline of how this could be implemented.

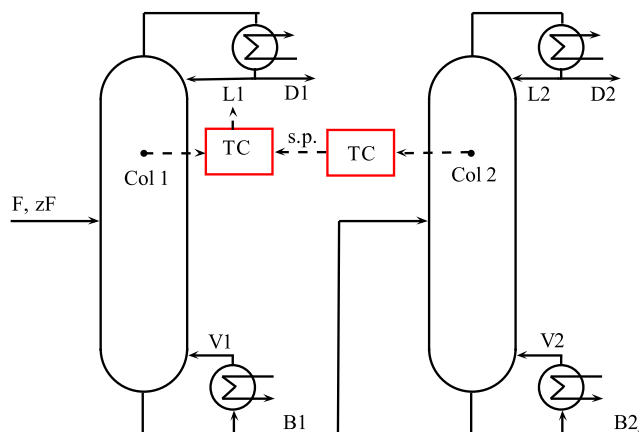


Figure 6.3.1: Proposed control structure for controlling a tray temperature in the top part of the second column by manipulating the reflux in column 1. The temperature in the second column is arranged in cascade with a local temperature loop in column 1.

Furthermore, the direct evaluation of loss indicated that also the concentration of component A in the bottom of the first column would be a good controlled variable.

As both steam flows are controlled at their maximum value, the steam cost would be constant. Thus the cost function can be reduced too the income from the three product flows. The price of the flows D_1 and B_1 , are both 1 \$/mol, and the price of the valuable product D_2 is 2 \$/mol. When the product specification of the valuable product is fixed, and the price of D_1 and B_1 is identical, the optimum

would be when the flow D_2 is at its maximum value. D_2 would be at maximum when the ratio between component A and C in top of the second column are constant. This ratio is highly dependent on the temperature in the top part of the second column as well as on the concentration of A leaving the first column. This would explain why these two variables were found to be good controlled variables.

6.3.1 Use of combination measurements

The "exact local method" shows that the use of combination of measurements would give a substantial reduction of loss in the case where only temperatures from the first column were selected. Controlling a combination of the three best tray temperatures would reduce the loss by 50 % as compared to controlling the temperature in the single best tray. However, even when a combination of 10 measurements in the first column, a single tray measurement in the top part of the second column would be substantially better.

Chapter 7

Conclusion

Two distillation columns in sequence were studied in order to identify the optimal control structure. A map of how the active constraint regions changes to variations in the steam price and the feed flow was found. The resulting map was close to the map found by Jacobsen [3], but showed some differences associated with constraint region borders.

Two of the regions were studied further in order to find self-optimizing variables. Both "direct evaluation of loss" and the "exact local method" were used to search for the controlled variables that would give the least loss. In the region with low energy cost, region VI, both methods found that controlling a tray in the top part of the second column would be the best choice if a single tray temperature should be controlled. Alternatively, the "direct evaluation of loss" indicated that the bottom concentration of component A would be a good controlled variable.

In the other region considered (region I), the "exact local method" was used to find the best set of three tray temperatures, selected from both columns, with respect to loss. The tray temperatures seemed to be located in areas with a good

trade-off between high gain and low optimal sensitivity, figure 5.4.1 and 5.4.2.

A systematic procedure to find the optimal control structure is outlined in the thesis. The procedure is designed to illustrate the main steps needed to develop a automated computer program for this part to column optimization.

7.1 Suggestions for future work

The present thesis address two topics. One concerns the optimization of two distillation columns in sequence and the other how to design a systematic procedure to find the optimal control structure.

The study of two distillation column has been limited to certain aspect of the problem. First, the active constraint region map has been found for only two disturbances. For a full understanding of the system, the active constraint regions should be found in all disturbance dimensions. Second, only three disturbances have been considered in the search for primary controlled variables. More disturbances should be considered. It should also be explored how the optimal primary controlled variables change within a constraint region and identify the optimal structure in other constraint regions.

In the thesis the active constraint regions are found by optimizing over a grid in the disturbance space. This approach needs substantial computational power. More efficient algorithms have to be developed before the active constraint region map can be found for a more complex system. An effort should also be made to develop algorithms for finding the primary controlled variables that gives the least loss within the boundaries of acceptable controllability.

In an active constraint region it is optimal to control the active constraints. To achieve this, the control structure needs to be changed when moving into another region. Further study should be conducted to develop methods for detecting when the system has made such change.

It is desirable to have as simple control structure as possible. It might be possible to find a control structure that give acceptable loss over several disturbance regions. This could be studied using any of the methods to calculate loss addressed in this thesis.

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Appendices

Appendix A

Linearization of the model using finite differences

The model was linearized around a nominal point. The linear relationship between the input, u , and output, y , is given by the matrix:

$$G = \frac{dy}{du} = \begin{pmatrix} \frac{\partial y_1}{\partial u_1} & \frac{\partial y_1}{\partial u_2} & \dots & \frac{\partial y_1}{\partial u_n} \\ \frac{\partial y_2}{\partial u_1} & \frac{\partial y_2}{\partial u_2} & \dots & \frac{\partial y_2}{\partial u_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial u_1} & \frac{\partial y_m}{\partial u_2} & \dots & \frac{\partial y_m}{\partial u_n} \end{pmatrix} \quad (\text{A.0.1})$$

Similarly, the linear relationship between the disturbance, d , and the output, y , is given by the matrix:

$$Gd = \frac{dy}{dd} = \begin{vmatrix} \frac{\partial y_1}{\partial d_1} & \frac{\partial y_1}{\partial d_2} & \cdots & \frac{\partial y_1}{\partial d_n} \\ \frac{\partial y_2}{\partial d_1} & \frac{\partial y_2}{\partial d_2} & \cdots & \frac{\partial y_2}{\partial d_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial y_m}{\partial d_1} & \frac{\partial y_m}{\partial d_2} & \cdots & \frac{\partial y_m}{\partial d_n} \end{vmatrix} \quad (\text{A.0.2})$$

The second derivative of the cost function with respect to inputs, J_{uu} (given by equation A.0.3) and the second derivative of the cost function with respect to input and disturbance, J_{ud} (given by A.0.4) where found by calculating either forward or backward differences. The general expressions for approximating the second derivative using forward and backward differences are given in equation A.0.5 and equation A.0.6, respectively [14].

$$J_{uu} = \frac{\partial^2 J}{\partial u \partial u} = \begin{vmatrix} \frac{\partial^2 J}{\partial u_1 \partial u_2} & \frac{\partial^2 J}{\partial u_1 \partial u_2} & \cdots & \frac{\partial^2 J}{\partial u_1 \partial u_n} \\ \frac{\partial^2 J}{\partial u_2 \partial u_2} & \frac{\partial^2 J}{\partial u_2 \partial u_2} & \cdots & \frac{\partial^2 J}{\partial u_2 \partial u_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 J}{\partial u_n \partial u_2} & \frac{\partial^2 J}{\partial u_n \partial u_2} & \cdots & \frac{\partial^2 J}{\partial u_n \partial u_n} \end{vmatrix} \quad (\text{A.0.3})$$

$$J_{ud} = \frac{\partial^2 J}{\partial u \partial d} = \begin{vmatrix} \frac{\partial^2 J}{\partial u_1 \partial d_2} & \frac{\partial^2 J}{\partial u_1 \partial d_2} & \cdots & \frac{\partial^2 J}{\partial u_1 \partial d_n} \\ \frac{\partial^2 J}{\partial u_2 \partial d_2} & \frac{\partial^2 J}{\partial u_2 \partial d_2} & \cdots & \frac{\partial^2 J}{\partial u_2 \partial d_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 J}{\partial u_n \partial d_2} & \frac{\partial^2 J}{\partial u_n \partial d_2} & \cdots & \frac{\partial^2 J}{\partial u_n \partial d_n} \end{vmatrix} \quad (\text{A.0.4})$$

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{f(x + h_i e_i + h_j e_j) - f(x + h_i e_i) - f(x + h_j e_j) + f(x)}{h_i h_j} \quad (\text{A.0.5})$$

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{f(x - h_i e_i - h_j e_j) - f(x - h_i e_i) - f(x - h_j e_j) + f(x)}{h_i h_j} \quad (\text{A.0.6})$$

It turned out to be difficult to find accurate values for the second derivatives J_{uu} and J_{ud} , see section B.2.

Appendix B

Validation of the linearization

B.1 Optimal sensitivity

The optimal sensitivity of the output with respect to the disturbance, F , may be found directly by perturbing the disturbance or using equation B.1.1.

$$F = -F^y J_{uu}^{-1} J_{ud} + G_d^y \quad (\text{B.1.1})$$

The optimal sensitivity found by linearizing the model by finite differences and using equation B.1.1, was compared to the optimal sensitivity found by perturbing the system directly. The comparison was done in order to validate the numerical accuracy of the linearization. The optimal sensitivity in the nominal point studied in region VI and I are given in figure B.1.1 and B.1.2, respectively. The individual points marked by dots were calculated using equation B.1.1, and the solid lines were calculated directly by perturbing the disturbances.

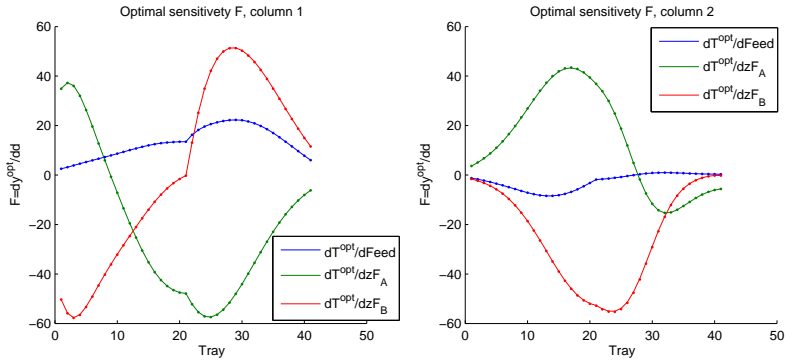


Figure B.1.1: The optimal sensitivity of the temperature with respect to three disturbances in constraint region IV. The individual points marked by dots were calculated using equation B.1.1, and the solid lines were calculated directly by perturbing the disturbances

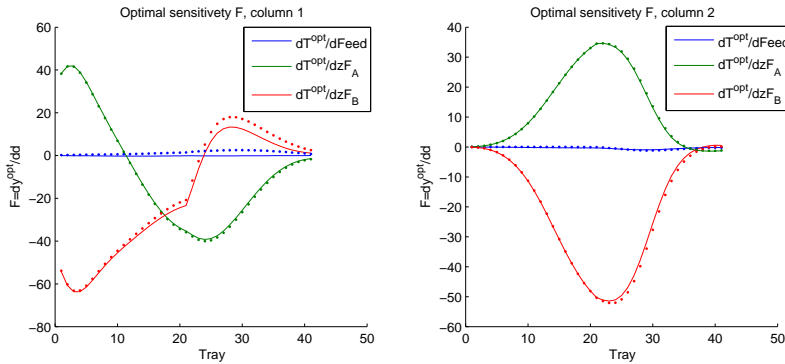


Figure B.1.2: The optimal sensitivity of the temperature with respect to three disturbances in constraint region I. The individual points marked by dots were calculated using equation B.1.1, and the solid lines were calculated directly by perturbing the disturbances

B.2 Validating J_{uu} and J_{ud} in region I

Numerical values for the derivatives J_{uu} and J_{ud} turned out to be difficult. Forward and backward differences were compared to validate the values. Numeric

values for J_{uu} and J_{ud} calculated using forward and backward differences, in the nominal point in region I, are given below.

$$J_{uu}_{forward} = \begin{bmatrix} 251.4575 & -256.9479 & -4.0768 \\ -256.9479 & 262.6072 & 4.1746 \\ -4.0768 & 4.1746 & 0.1630 \end{bmatrix} \quad (\text{B.2.1})$$

$$J_{uu}_{backwards} = \begin{bmatrix} 248.8970 & -256.9845 & -4.0602 \\ -256.9845 & 265.3887 & 4.1928 \\ -4.0602 & 4.1928 & 0.1630 \end{bmatrix} \quad (\text{B.2.2})$$

$$J_{ud}_{forward} = \begin{bmatrix} 128.9938 & 332.2961 & 33.8723 \\ -131.9673 & -339.4311 & -34.8896 \\ -2.2638 & -4.8811 & -0.7721 \end{bmatrix} \quad (\text{B.2.3})$$

$$J_{ud}_{backwards} = \begin{bmatrix} 128.0086 & 328.2654 & 33.6873 \\ -132.3138 & -338.8721 & -35.0375 \\ -2.2594 & -4.8522 & -0.7717 \end{bmatrix} \quad (\text{B.2.4})$$

Appendix C

Matlab scripts

This chapter present the most relevant Matlab scripts used in the project. An overview of the scripts used in the thesis shown in table C.0.1. All scripts presented in the table are given in the subsequent sections except "linerize.m" and "Fmat.m"

Table C.0.1: Overview of the scripts used in the thesis

Script name	Description
Active constraint region map	
constraintplot.m	Finds the active constraint region maps
binary.m	Marks the active set as a binary number
Direct evaluation	
brute_force.m	Direct evaluation of loss
global_direct_evaluation.m	Global direct evaluation of loss
Exact local method	
Run_exact_local_metod.m	Uses the "exact local method" to find the optimal combination of measurements
exact_local_method.m	Calculates the matrix H based on the analytical expression of the "exact local method".
Model	
multiCP_ColumnA_ext.m	Steady state model of column A
Temp.m	Approximates temperature based on composition
nonlcon.m	Nonlinear constraints in the system
init_nominal.m	Initial condition to the model and optimization
Gain and optimal sensitivity	
linerize.m	Calculates G^y , G_d^y , J_{uu} and J_{ud}
Fmat.m	Calculates the optimal sensitivity by direct perturbation

C.1 Search for the active constraint region active constraint region

The script "constraintplot.m" attempts to find the active constraint region map by optimizing in a grid over the specified disturbance space. The function "binary.m" mark the active set as a binary number.

constraintplot.m

```
1 %% constraintplot.m
2 % Summary:      Finds the active constraint regions in a
3 %              userspecified disturbance space. Default is
4 %              Feed vs price of steam.
5 %
6 %              The disturbance space is found by optimise
7 %              in all point i a grid of the disturace space.
8 %              The active set each point is marked by a
9 %              binary number.
10 %
11 % author:      Tor Anders Marvik
12 % organization: Department of Chemical Engineering, NTNU, Norway
13 % contact:     torandma@stud.ntnu.no
14 % started     Oktober 2012
15
16 clc
17 clear all
18
19 %Intial values
20 init_nominal           % Initial values
21 load('xopt_F14_pV001') % Load nominal optimum
22 x0=xopt;              % Initial guess
23
24 %Nominal point
25 par.F=1.4;
26 price.steam=0.01;
27
28 % Calculating optimal point
29 par.flag=0;           % No control
30 par.actset=[];       % No active constraints
31
32 [x_opt,fval_opt,exitflag]=fmincon(@(x) costfunction(...
33     x,price,par),x0,[],[],[],[],lb,ub,@(X)nonlcon(...
34     X, par),options);
```

```

35 [Toptcol1,Toptcol2] = Temp(x_opt,par);
36 Topt=[Toptcol1;Toptcol2];           % Optimal temperatures
37
38 % Solver options
39 options = optimset('TolFun',10e-6,'TolCon',10e-6,...
40                   'MaxFunEvals',5e3,'Display','off','Algorithm',...
41                   'sqp','Diagnostics','off');
42
43 %constraints
44 tol=1e-6;                           % Tolerance from constraint
45
46 % Resolution on x and y axis
47 n_x=20;                               % Resolution on the x axis
48 n_y=20;                               % Resolution on the y axis
49
50 % Choose disturbance space
51 x_grid=linspace(1.35,1.495,n_x); % Grid disturbance on x axis
52 y_grid=linspace(0.01,0.19,n_y); % Grid disturbance on y axis
53
54 %Solver conditions
55 par.flag=0;                           % No control=0, Xcont=1,...
56 par.actset=[];                         % No controlled active const.
57
58 %Init matrices
59 val=zeros(n_x*n_y,9);                 % Init [bin exitflag fval,x,y]
60 fval_mat=zeros(n_x*n_y,2);           % Init const value matrix
61 x_mat=zeros(n_x*n_y,2*par.NV+8); % init x data matrix
62
63 exitflag=1;                           % Convergence flag
64 k=0;                                   % Count progression
65 time=0;                                % Monitor time
66
67 for i=1:n_x                             % Loop x axis
68     par.F=x_grid(i);                   % Variable x axis
69
70     for j=1:n_y                           % Loop Y axis
71         tic                               % start time

```

```

72         k=k+1;                               % point number
73
74         price.steam=y_grid(j); % Variable X axis
75
76         %run fmincon
77         [x,fval,exitflag]=fmincon(@ (x) costfunction(...
78             x,price,par),x0,[],[],[],[],lb,ub,...
79             @(X) nonlcon(X,par),options);
80
81         % Constraint valus at optimum
82         c=[x(par.NV+2),x(2*par.NV+6),x(par.NT),...
83             x(par.NV+4+2*par.NT),x(par.NV+4+2*par.NT+1)];
84
85         if exitflag == 1           % Warm start
86             x0=x;
87         end
88
89         bin= binary(c,c_s,tol); % Marke active set as bin num
90
91         val(k,:)= [bin,exitflag,fval,y_grid(1,j),x_grid(i)];
92
93         % Monitor progression
94         disp([k , val(k,:),toc])
95         time=time+toc;
96
97         %save date for other functions
98         x_mat(k,:)=x';
99         fval_mat(k,:)=fval;
100        points(i,j,:)= [x;fval;x_grid(i);y_grid(j);exitflag];
101
102    end
103 end
104
105 % save data for other funtions
106 data.n_x=n_x;
107 data.n_y=n_y;
108 data.val=val;

```

```

109 data.x_mat=x_mat;
110 data.fval_mat=x_mat;
111
112 time;                               % Total time
113
114 % Plot contourplot
115 figure(1)
116 hold on
117
118 contour(x_grid,y_grid(1,:), reshape(val(:,1),n_x,n_y), [1],...
119         'Color', rgb('Orange'),'LineWidth',2);
120 contour(x_grid,y_grid(1,:), reshape(val(:,2),n_x,n_y), [1],...
121         'Color', rgb('Blue'),'LineWidth',1);
122 contour(x_grid,y_grid(1,:), reshape(val(:,3),n_x,n_y), [1],...
123         'Color', rgb('Red'),'LineWidth',2);
124 contour(x_grid,y_grid(1,:), reshape(val(:,4),n_x,n_y), [1],...
125         'Color', rgb('Purple'),'LineWidth',2);
126 contour(x_grid,y_grid(1,:), reshape(val(:,5),n_x,n_y), [1],...
127         'Color', rgb('Green'),'LineWidth',2);

```

binary.m

```

1 function [bin] = binary (c,c_s,tol)
2 %% binary.m
3 % Summary:      Compare the state of the system with the
4 %              constraints c_s and mark the active set a
5 %              binary number.
6 % author:      Tor Anders Marvik
7 % organization: Department of Chemical Engineering, NTNU,
8 % contact:     torandma@stud.ntnu.no
9 % Input        c    : constraint variable at optimal point
10 %             c_s  : constraint values
11 %             tol  : Toleranse, active constr. if c-c_s <tol
12 % Output      bin  : Binary number that marks the active set

```

```
13
14
15 bin=zeros(1,5);
16
17 for i=1:5
18     if abs(c(i)-c_s(i))<tol
19         bin(i)=1;
20     end
21 end
22
23 end
```

C.2 Self optimizing variables

C.2.1 Direct evaluation

brute_force.m

```
1 %% brute_force.m
2 % Summary:      Direct evalutaion of loss for a selection of
3 %              variables held
4 %              constant
5 % author:      Tor Anders Marvik
6 % organization: Department of Chemical Engineering, NTNU, Norway
7 % contact:     torandma@stud.ntnu.no
8 % requires:    matlab
9 % version:     1.0
10 % todo 1.0:   Debugging "There is always a second bug"
11 % started     Oktober 2013
12 %%
13
14
```

```

15  init_nominal          % initial values for the optimization
16  load('xopt_F14_pV001')
17  % ----- Optimize in nominal point -----
18  par.actset=[]; % No active constraints
19  par.flag=0; % No control
20  [x_opt,fval_opt,exitflag]=fmincon(@(x) ...
21      costfunction(x,price,par),x0,[],[],[],[],...
22      lb,ub,@(X)nonlcon(X,par),options);
23  [Toptcol1,Toptcol2] = Temp(x_opt,par);
24  T_opt=[Toptcol1;Toptcol2];
25  x0=x_opt;
26
27  % ----- Initial loss vectors -----
28  Loss_T=zeros(1,41); % Loss vektor, temp from col1 const.
29  Loss_T_col2=zeros(1,41); % Loss vektor, temp from col2 const.
30  Loss_x=zeros(1,4); % Loss vektor, a variable in x const.
31  Loss_F=zeros(1,2); % Loss vektor when a ratio with F const.
32  Loss_comb=zeros(1,1); % Loss when L1/D1 constant
33
34  % ----- Insert the disturbance -----
35  k=1; % For global direct evaluation
36  par.F=1.4;
37  par.zF=[0.4 0.2 4]';
38  par.qF=1.0;
39  price.pD1=1.0;
40
41  % ----- Reoptimize -----
42  par.actset=[]; % no active constraints
43  par.flag=0;
44  [x_reopt,fval_reopt,exitflag]=fmincon(@(x) ...
45      costfunction(x,price,par),x0,[],[],[],[],...
46      lb,ub,@(X)nonlcon(X,par),options);
47
48  [Treoptcol1,Treoptcol2] = Temp(x_reopt,par);
49
50  % ----- Calculation the loss -----
51  % Flag = 1: x() controlled

```

```

52 % Flag = 2: A temperature in column 1 controlled
53 % Flag = 3 x1()/x2() controlled
54 % Flag = 4 x()/F() controlled
55
56 par.flag=1; %Keeping variable in x constant
57 par.actset=[]; % No active constraints
58
59 index_x=[ par.NV+1;... % L1 % coordinate in x for CV used
60           par.NV+3;... % D1
61           1;... % xb_A
62           41]; % xd_A
63
64 for i=1:length(index_x)
65     par.index_u=index_x(i);
66     par.dof=x_opt(par.index_u); % s.p. for the CV
67     [x,fval,exitflag]=fmincon(@(x) costfunction(x,price,par),...
68     x0,[],[],[],[],lb,ub,@(X) nonlcon(X,par),options);
69     if exitflag<0 % no solutions found?
70         Loss_x(k,i)=inf
71     else
72         Loss_x(k,i)=fval-fval_reopt(k,:) % The loss
73     end
74 end
75
76 par.flag=2; % Keeping variable in T constant
77 par.actset=[]; % No active constraints
78
79 index_T=1:41;
80 for i=[1,10,20,30,41]
81     par.index_u=index_T(i);
82     par.dof=T_opt(par.index_u); % s.p. for the CV
83     [x,fval,exitflag]=fmincon(@(x) costfunction(x,price,par),...
84     x0,[],[],[],[],lb,ub,@(X) nonlcon(X,par),options);
85     if exitflag<0 % no solutions found
86         Loss_T(k,i)=inf
87     else
88         Loss_T(k,i)=fval-fval_reopt(k,:) % The loss

```

```

89     end
90 end
91
92 par.flag=3;           % Keeping variable in T constant
93 par.actset=[];       % No active constraints
94 index_comb=[ par.NV+1,par.NV+3 ]; % [L1 D1]
95
96 for i=1:size(index_comb,1)
97     par.index_u=index_comb(i,:);
98     par.dof=x_opt(par.index_u(1))/x_opt(par.index_u(2));
99     [x,fval,exitflag]=fmincon(@(x) costfunction(x,price,par),...
100         x0,[],[],[],[],lb,ub,@(X) nonlcon(X,par),options);
101     if exitflag<0      % no solutions found?
102         Loss_comb(k,i)=inf
103     else
104         Loss_comb(k,i)=fval-fval_reopt(k,:) % The loss
105     end
106 end
107
108 par.flag=4;          %Keeping variable in T constant
109 par.actset=[];      % no active constraints
110 index_F=            [par.NV+3;... % D1/F
111                    par.NV+1]; % L1/F
112
113 for i=1:length(index_F)
114     par.index_u=index_F(i);
115     par.dof=x_opt(par.index_u)/par.F; % s.p. for the CV
116     [x,fval,exitflag]=fmincon(@(x) costfunction(x,price,par),...
117         x0,[],[],[],[],lb,ub,@(X) nonlcon(X,par),options);
118     if exitflag<0      % no solutions found, infeasible?
119         Loss_F(k,i)=inf
120     else
121         Loss_F(k,i)=fval-fval_reopt(k,:) % The loss
122     end
123 end
124
125 % Temperature column 2

```



```

126 par.flag=2; % Keeping variable in T constant
127 par.actset=[]; % No active constraints
128
129 index_T=1:41;
130 for i=1:41
131     par.index_u=index_T(i)+41;
132     par.dof=T_opt(par.index_u);
133     [x,fval,exitflag]=fmincon(@(x) costfunction(x,price,par),...
134         x0,[],[],[],[],lb,ub,@(X) nonlcon(X,par),options);
135     if exitflag<0 % no solutions found
136         Loss_T_col2(k,i)=inf
137     else
138         Loss_T_col2(k,i)=fval-fval_reopt(k,:) % The loss
139     end
140 end
141
142
143 % Selected loss velues [Loss*1000]
144 Loss_selction=[Loss_x(1,:)';Loss_T([1,10,20,30,41])';...
145     Loss_F';Loss_comb';Loss_T_col2([1,10,20,30,41])']*1000
146
147 %Reoptimised cv values
148 CV_opt=[x_reopt(index_x);Treoptcol1([1,10,20,30,41]);...
149     x_reopt(par.NV+3)/par.F;x_reopt(par.NV+1)/par.F;...
150     x_reopt(par.NV+1)/x_reopt(par.NV+3);...
151     Treoptcol2([1,10,20,30,41])]

```

C.2.2 Global direct evaluation of loss

controlled_line.m

```

1 %% controlled_line.m
2 % Summary: The script calcualtes a loss when controlling
3 % the system and increasing and decreasing a

```

```

4 %           disturbance from nominal
5 % author:   Tor Anders Marvik
6 % organization: Department of Chemical Engineering, NTNU, Norway
7 % contact:  torandma@stud.ntnu.no
8
9 clc
10 clear all
11
12 init_nominal           % initial values
13
14 %Nominal point
15 par.F=1.4;
16 price.steam=0.01;
17
18 %calculating nominal optimum
19 par.flag=0;           % No control
20 par.actset=[];       % No active constraints
21
22 [x_opt,fval_opt,exitflag]=fmincon(@(x) costfunction(...
23                               x,price,par),x0,[],[],[],[],lb,ub,@(...
24                               X)nonlcon(X, par),options);
25 [Toptcol1,Toptcol2] = Temp(x_opt,par);
26 T_opt=[Toptcol1;Toptcol2]; % Temperature at optimum
27
28 zF=[];               % Initiate composition vector
29 F=[];               % Initiate feed vektor
30
31
32 par.flag=2; %0= no cont., 1 = cont. variable in x, 2 = cont. T
33 par.actset=[1;2;4]; % Index of active constraints
34 par.index_u=41+41; % Index controlled variable
35 par.dof=T_opt(par.index_u);
36
37 i=1;
38 exitflag=1;
39 while par.F>1.35 && exitflag>=0
40     par.F=par.F-0.001; % disturbance step

```

```

41
42     %calculate optimum
43     par.actset=[];
44     par.flag=0;           % No control
45     [x_reopt(:,i),fval_reopt(i),exitflag]=fmincon(@(x)...
46             costfunction(x,price,par), x0,[],[],[],[],...
47             lb,ub,@(X)nonlcon(X, par),options);
48
49     %calculate controlled
50     par.actset=[1;2;4]; % index of active constraints
51     par.flag=2;
52     [x(:,i),fval(i),exitflag]=fmincon(@(x) ...
53             costfunction(x,price,par),x0,[],[],[],[],...
54             lb,ub,@(X)nonlcon(X, par),options);
55     exitflag
56
57     zF(:,i)=par.zF;
58     F(i)=par.F
59     steam(i)=price.steam;
60     x0=x(:,i);
61     i=i+1;
62 end
63
64 F=fliplr(F);
65 zF=fliplr(zF);
66 x=fliplr(x);
67 fval=fliplr(fval);
68 steam=fliplr(steam);
69 x_reopt=fliplr(x_reopt);
70 fval_reopt=fliplr(fval_reopt);
71
72 %reset initial conditoinis
73 par.dof=T_opt(par.index_u);
74 exitflag=1;
75 par.F=1.4;
76 par.zF=[0.4,0.2,0.4]';
77 price.steam=0.01;

```

```

78
79 while par.F<1.5 && exitflag>=0
80     par.F=par.F+0.001;           % disturbance step
81
82     %calculate optimum
83     par.flag=0;                   % no control
84     par.actset=[];
85     [x_reopt(:,i),fval_reopt(i),exitflag]=fmincon(@(x)...
86         costfunction(x,price,par),x0,[],[],[],[],...
87         lb,ub,@(X) nonlcon(X, par),options);
88
89     %calculate controlled
90     par.flag=2;
91     par.actset=[1;2;4]; % index of active constraints
92     [x(:,i),fval(i),exitflag]=fmincon(@(x)...
93         costfunction(x,price,par), x0,[],[],[],[],...
94         lb,ub,@(X) nonlcon(X, par),options);
95
96     zF(:,i)=par.zF;
97     F(i)=par.F
98     steam(i)=price.steam;
99     x0=x(:,i);
100    i=i+1;
101 end
102
103
104 F=F(2:end-1); %first and last element is infeasible
105 zF=zF(:,2:end-1); %first and last element is infeasible
106 x=x(:,2:end-1); %first and last element is infeasible
107 fval=fval(2:end-1);
108 x_reopt=x_reopt(:,2:end-1);
109 fval_reopt=fval_reopt(2:end-1);
110 steam=steam(2:end-1);
111 Loss=fval-fval_reopt;
112
113
114 %save()

```

C.2.3 The "exact local method"

Run_exact_local_metod.m

```
1
2 % Summary:      Linerize the model and find the optimal
3 %               control variables base on exact local methode.
4 % author:      Tor Anders Marvik
5 % organization: Department of Chemical Engineering, NTNU,
6 % contact:     torandma@stud.ntnu.no
7
8 init_nominal;  % Initialize nominal conditioins
9
10 % Initial point
11 Feed=1.35;    % Nominal feed
12 steam=0.03;  % Nominal steam price
13
14 % Active set
15 actset=[4]; % set of active constraints [V1,V2, x_A, x_B, X_C]
16 index_u=[par.NV+1;par.NV+2;2*par.NV+6]; % Index of MV's in x
17
18 du=[0.00001]; % Pertubation step in manipulated variables
19 dd=[0.00001]; % Pertubation step in disturbances
20
21 % Linerize model
22 [G1,Gd,Juu,Jud,exitflag]=linerize(...
23                               index_u,actset,du,dd,Feed,steam);
24
25 % Measurement and implementation error
26 Wd=diag([0.01,;0.01;0.01]);% Magnitude of expected disturbance
27 Wn=diag(ones(82,1)*0.5); % Meassurement error ny*ny
28
29 % Run a version of the brance and bound:
30 % - Single measurements: b3av or b3wc
31 % - Combinations of measurements: pb3av or pb3av
```

```

32
33 % Running b3av and b3wc
34 G_comb=[G1.dTcol1du;G1.dTcol2du]; % Process model
35 Gd1=[Gd.dTcol1dd;Gd.dTcol2dd]; % Disturbance model
36
37 [B,sset,ops,ctime,flag]=b3av(G_comb,Gd1,Wd,Wn,...
38     Juu.av,Jud.av,inf,200);
39 % An error in the algoritgm causes infeasible
40 % values with loss -inf to be sorted fist in B
41 % and sset: Fist feasible values given by:
42 k=1;
43 while B(k)<0
44     k=k+1;
45 end
46 B=B(k:end,:);
47 sset=sset(k:end,:);
48
49 % Use exact local methode directly -----
50
51 [H,loss_av,loss_wc,loss_av_cao,loss_wc_cao]=...
52 exact_local_method(sset(1,:),G_comb,Gd1,Wd,Wn,Juu.av,Jud.av);

```

exact_local_method.m

```

1 %% exact_local_methode.m
2 % Summary: The script calculate H matrix and loss using
3 % the analytic soultion to the exact local methode.
4 % The H matrixgives the optimal combinations of
5 % mesurement to be controlled with the measurement
6 % and implementation error considered.
7 %
8 % author: Tor Anders Marvik
9 % org.: Department of Chemical Engineering, NTNU, Norway
10 % contact: torandma@stud.ntnu.no

```

```

11 % started      Oktober 2012
12
13
14 function [H,loss_av,loss_wc,loss_av_cao,loss_wc_cao]=...
15     exact_local_method(sset,G_comb,Gd1,Wd,Wn,Juu,Jud)
16
17 %select a subset of G1,Gd,Juu,Jud
18 G1_ss=G_comb(sset(1,:),:);
19 Gd_ss=Gd1(sset(1,:),:);
20 Wd_ss=Wd;                                     % Magnitude disturbance
21 Wn_ss=Wn(sset(1,:),sset(1,:)); % Weighting of the noise
22
23 ny=length(sset);                             % Number of measurements
24 nd=3;                                         % Number of disturbances
25 F_ss=-G1_ss*(Juu)^-1*Jud+Gd_ss;
26 Y=[F_ss*Wd_ss' Wn_ss];
27
28 H=(inv(Y*Y')*G1_ss*inv(G1_ss'*inv(Y*Y')*G1_ss)*sqrtm(Juu))';
29
30 %Loss
31 M=sqrtm(Juu)*inv(H*G1_ss)*H*Y;
32 loss_wc=0.5*svds(M,1)^2 ;
33 loss_av=0.5*norm(M,'fro')^2;
34
35 %worst case loss alternative
36 G=G1_ss*inv(sqrtm(Juu));
37 Y2=Y*Y';
38 X=chol(Y2)\G;
39 lambda=eig(X'*X);
40 Loss_wc2=0.5./min(lambda);
41
42 %average loss alternative, uniform distribution
43 G=G1_ss*inv(sqrtm(Juu));
44 Y2=Y*Y';
45 X=chol(Y2)\G;
46 lambda=eig(X'*X);
47 loss_wc_cao=0.5./min(lambda);

```

```

48
49 G2=G*G';
50 [R,f]=chol(G2);
51 X=R'\Y;
52 lambda=sum(sum(X.*X));
53 loss_av_cao=sort(lambda/(6*(size(Wd,2)+1)));
54
55 end

```

C.3 The model

The model is a steady state version of column A [15], handling multiple components.

The script `multiCP_ColumnA_ext.m` is a model of a single column. The model is implemented in the optimization problem as nonlinear equality constraints in the script `nonlcon.m`. The tray temperatures are given by the function `Temp.m` and the initial condition is provided by `init_nominal.m`

C.3.1 Steady state model of column A

`multiCP_ColumnA_ext.m`

```

1 function [ residue] = multiCP_ColumnA_ext( X,par )
2 %
3 %           This is a nonlinear steady state model of a
4 %           multicomponent distillation column with
5 %           NT-1 theoretical stages including a reboiler
6 %           (stage 1) plus a total condenser ("stage" NT).
7 %
8 %           Model assumptions:

```



```

9 %
10 %           Two components (binary separation);
11 %           Constant relative volatility;
12 %           No vapor holdup;
13 %           One feed and two products;
14 %           Constant molar flows (same vapor flow on all
15 %           stages);
16 %           Total condenser
17 %
18 %           The model is based on column A in Skogestad and
19 %           Postlethwaite (1996). The model has NT*NC states.
20 %
21 % Inputs:      x - states, the NT*NC compositions
22 %               reboiler/bottom stage as x(1,i) and condenser
23 %               as x(NT,i) .
24 %           par.LT      - reflux L,
25 %           par.VB      - boilup V,
26 %           par.D       - top or distillate product flow D,
27 %           par.B       - bottom product flow B,
28 %           par.F       - feed rate F,
29 %           par.zF      - feed composition, zF.
30 %           par.qF      - feed liquid fraction, qF.
31 %           par.NT      - number of stages, NT.
32 %           par.NF      - location of feed stage, NF.
33 %           par.alpha   - relative volatilities, alpha.
34 %           par.NC      - number of components,NC.
35 %
36 % Outputs:    [residue] = f(x), residue=0 if x is a solution of
37 %             the system of nonlinear equations
38
39 %-----
40
41 % Inputs and disturbances
42 LT = par.LT;           % Reflux
43 VB = par.VB;           % Boilup
44 D  = par.D;            % Distillate
45 B  = par.B;            % Bottoms

```

```

46
47 F = par.F;           % Feedrate
48 zF = par.zF;        % Feed composition
49 qF = par.qF;        % Feed liquid fraction
50
51 NT = par.NT;        % Number of stages
52 NF = par.NF;        % Location of feed stage
53 alpha = par.alpha;  % Relative volatility
54 NC = par.NC;        % Number of components
55
56 %Preallocation
57 %y=ones(NT-1,NC-1);
58 dMxdt = ones(NT,NC-1);
59 dMdt = ones(2,1);
60 x=X(1:NT*(NC-1));
61 x=reshape(x,NT,NC-1);
62 % THE MODEL
63
64 % Vapor-liquid equilibria
65 y = (x*diag(alpha(1:NC-1)))./((x*(alpha(1:NC-1) - 1) + 1)*...
66     ones(1,NC-1));
67 % -----Column-----
68 %
69 % Component balances
70 % =====
71 % Reboiler (assumed to be an equilibrium stage)
72 i = 1:NC-1;
73 dMxdt(1,i) = (LT+qF*F)*x(2,i) - VB*y(1,i) - B*x(1,i);
74 % Stripping section trays
75 j=2:NF-1;
76 dMxdt(j,i) = (LT+qF*F)*x(j+1,i) - (LT+qF*F)*x(j,i) + ...
77     VB*y(j-1,i) - VB*y(j,i);
78 % Feed tray
79 dMxdt(NF,i) = LT*x(NF+1,i) - (LT+qF*F)*x(NF,i) + ...
80     VB*y(NF-1,i) - (VB+(1-qF)*F)*y(NF,i) + F*zF(i)';
81 % Enrichment section trays
82 j=NF+1:NT-1;

```

```

83 dMxdt(j,i) = (LT)*x(j+1,i) - LT*x(j,i) + (VB+(1-qF)*F)*y(j-1,i) ...
84             - (VB+(1-qF)*F)*y(j,i);
85 % Total condenser (no equilibrium stage)
86 dMxdt(NT,i) = (VB+(1-qF)*F)*y(NT-1,i) - LT*x(NT,i) - D*x(NT,i);
87 %=====
88 % Mass balances
89 %=====
90 % Reboiler
91 dMdt(1) = LT+qF*F      - VB      - B;
92 % Condenser
93 dMdt(2) = VB+(1-qF)*F - LT      - D;
94 % =====
95 % Summation Balances
96 % =====
97 Xs=reshape(X,NT,NC);
98 sumXs=1-Xs*ones(NC,1);
99 %
100 %-----
101 %
102 %
103 % Output
104 residue=[dMxdt(:); dMdt; sumXs(:)];

```

C.3.2 Temperature estimator

```

1 function [Tcol1,Tcol2] = Temp(x,par)
2 %% Temp.m
3 % Summary:
4 % Tray temperature estimator for column 1 and column 2
5 % The temperature is based on a linear relation between the
6 % boiling points of the pure components.
7 %
8 % Boiling point assumptions
9 %           Tb_A=30 *C

```

```

10 %           Tb_B=70 *C
11 %           Tb_C=100 *C
12 %
13 % author:      Tor Anders Marvik
14 % organization: Department of Chemical Engineering, NTNU
15 % contact:     torandma@stud.ntnu.no
16 % input       x           : condition vektor
17 %            par        : Parameter struct
18 % Output      Tcol1      : Tray temperature vektor column 1
19 %            Tcol2      : Tray temperature vektor column 2
20
21 % Temperature function
22 T=@(x) 100-x(:,2)*(100-70)-x(:,1)*(100-30);
23
24 % Tray compositoin matrices
25 xcol1=[x(1:par.NT), ...
26        x(par.NT+1:2*par.NT), ...
27        x(2*par.NT+1:3*par.NT)];
28 xcol2=[x(par.NV+5:par.NV+4+par.NT), ...
29        x(par.NV+5+par.NT:par.NV+4+2*par.NT), ...
30        x(par.NV+5+2*par.NT:par.NV+4+3*par.NT)];
31
32 Tcol1=T(xcol1);           % Tray temperatures column 1
33 Tcol2=T(xcol2);           % Tray temperatures column 2
34
35
36 end

```

C.3.3 The nonlinear constraints

```

1 function [ c, ceq ] = nonlcon( x, par )
2
3 c=[];           %inequality constraints
4

```

```

5 par1=par;           %reseting struct parameters for coll
6 par2=par;           %reseting struct parameters for coll
7
8 %column 1
9 par1.F=par.F;
10 par1.zF=par.zF;
11 par1.LT=x(par.NV+1);
12 par1.VB=x(par.NV+2);
13 par1.D=x(par.NV+3);
14 par1.B=x(par.NV+4);
15 ceq_coll=multiCP_ColumnA_ext(x(1:par.NV),par1);
16
17 %column 2
18 par2.F=x(par.NV+4);
19 par2.zF=x([1,par.NT+1,2*par.NT+1]);
20 par2.LT=x(par.NV*2+4+1);
21 par2.VB=x(par.NV*2+4+2);
22 par2.D= x(par.NV*2+4+3);
23 par2.B= x(par.NV*2+4+4);
24 ceq_col2=multiCP_ColumnA_ext(x(par.NV+5:par.NV*2+4),par2);
25
26 %active constraints
27 act(1)=x(par.NV+2)-4.008;%           % Max vapour flow coll
28 act(2)=x(2*par.NV+6)-2.405;         % Max vapour flow col2
29 act(3)=x(par.NT)-0.95;              % Min comp A top coll
30 act(4)=x(par.NV+4+2*par.NT)-0.95;   % Min comp B top col2
31 act(5)=x(par.NV+4+2*par.NT+1)-0.95; % Min comp C btm col2
32 active=act(par.actset)';           % Set of acitive const.
33
34
35 if par.flag==0;                     % No control
36 ceq=[ceq_coll;ceq_col2;active];
37 else                                 % With control
38
39
40 dof=par.dof;                         % Setpoint contr. var.
41

```

```
42 %value in x vektor controlled
43 if par.flag==1
44     res_dof=x(par.index_u)-dof;
45     ceq=[ceq_col1;ceq_col2;active;res_dof];
46 end
47
48 %Tray temp controlled controlled
49 if par.flag==2
50     [Tcol1,Tcol2] = Temp(x,par);
51     T=[Tcol1;Tcol2];
52     res_dof=T(par.index_u)-dof;
53     ceq=[ceq_col1;ceq_col2;active;res_dof];
54 end
55
56 %x()/x() controlled
57 if par.flag==3
58     res_dof=x(par.index_u(1, 1))/x(par.index_u(1,2))-dof;
59     ceq=[ceq_col1;ceq_col2;active;res_dof];
60 end
61
62 %x()/F() controlled
63 if par.flag==4
64     res_dof=(x(par.index_u)/par.F)-dof;
65     ceq=[ceq_col1;ceq_col2;active;res_dof];
66 end
67
68 %c= H * T controlled
69 if par.flag==5;
70     [Tcol1,Tcol2] = Temp(x,par);
71     T=[Tcol1;Tcol2];
72     res_dof=par.H*T(par.index_u)-dof;
73     ceq=[ceq_col1;ceq_col2;active;res_dof];
74 end
75
76 end
77 end
```

C.3.4 Initial condition for a nominal point

```

1  % Initial conditions for the optimization problem
2  % default nominal point is F=1.4 and steam 0.01
3
4  %This script contains inital values
5
6  %intial values
7  par.F=1.4;                               % Feed flow rate
8  par.zF=[0.4 0.2 0.4]';                 % Feed composition
9  par.qF=1.0;                             % Feed liquid fraction
10 par.NC=3;                               % Number of components
11 par.NT=41;                              % Number of trays
12 par.NF=21;                              % Feed tray number
13 par.alpha=[2 1.5 1]';                 % Relative volatility
14
15 %Prices for the cost funciton
16 price.pF1=1;                           % Feed price col. 1
17 price.pD1=1;                           % Top product price col. 1
18 price.pD2=2;                           % Top product price col. 2
19 price.pB2=1;                           % Btm product price col. 2
20 price.steam=0.01;                      % vapour cost
21
22 %Number of decision variables
23 par.NV=par.NT*par.NC;                  % Number cons. decition var
24
25 %Define the constraint limits
26 V1max=4.008;                          % Max vapour flow col1
27 V2max=2.405;                          % Max vapour flow col2
28 Xd1Amin=0.95;                         % Min comp A top col1
29 Xd2Bmin=0.95;                         % Min comp B top col2
30 Xb2Cmin=0.95;                         % Max vapour flow col2
31
32
33 c_s=[V1max V2max Xd1Amin Xd2Bmin Xb2Cmin]; %constraints
34

```

```

35 %Initial Values
36 x0_col1=[ linspace(0.01,0.99,par.NT) ' ;
37           linspace(0.39,0.005,par.NT) ' ;
38           linspace(0.6,0.005,par.NT) ' ;
39           par.F/2;
40           par.F/2;
41           par.F/2;
42           par.F/2] ;
43 x0_col2=[ linspace(0.00,0.00,par.NT) ' ;
44           linspace(0.01,0.99,par.NT) ' ;
45           linspace(0.99,0.01,par.NT) ' ;
46           par.F/4;
47           par.F/4;
48           par.F/4;
49           par.F/4] ;
50
51 x0=[x0_col1;x0_col2];
52
53
54 %Define the lower and upper bounds
55 lb_col1=zeros((par.NV+4),1);
56 ub_col1=[ones(par.NV,1); [20 20 20 20]'];
57 lb_col2=zeros((par.NV+4),1);
58 ub_col2=[ones(par.NV,1); [20 20 20 20]'];
59
60
61 %Define constraints through lower and upper bounds
62 lb_col1(par.NT)=Xd1Amin;           % Min comp A top col1
63 lb_col2(2*par.NT)=Xd2Bmin;       % Min comp B top col2
64 lb_col2(2*par.NT+1)=Xb2Cmin;     % Min comp C btm col2
65 ub_col1(par.NV+2)=V1max;         % Max vapour flow col1
66 ub_col2(par.NV+2)=V2max;         % Max vapour flow col2
67
68 lb=[lb_col1;lb_col2 ];           % Lower bounds
69 ub=[ub_col1;ub_col2 ];           % Upper bounds
70
71

```



```
72 %fmincon options
73 options = optimset('TolFun',10e-8,'TolCon',10e-8,...
74     'MaxFunEvals',1e4,'Display','off','Algorithm',...
75     'sqp','Diagnostics','off');
76
77
78 T=@(x)100-x(:,2)*(100-70)-x(:,1)*(100-30); % Temp. estimator
```