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# Self-Optimizing Control Structures for Active Constraint Regions of a Sequence of Distillation Columns

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# Abstract

Investigating and mapping active constraint regions for processes, and subsequently finding control structures for each region, is vital for their optimal operation. In this work, active constraint regions of three different case studies for the distillation process have been investigated:

- A single distillation column with constant product prices.
- A single distillation column with purity dependent prices.
- Two distillation columns in sequence with constant prices.

The active constraint regions for each case study have been identified and mapped with respect to the disturbances; energy price and feed flow rate. Selected stage temperatures and combinations of stage temperatures have been proposed as self – optimizing variables for the unconstrained degrees of freedom of each region. These were found by the use of the Minimum Singular Value Rule and the Exact Local Method. The methods requires the optimal sensitivities of measurements with respect to disturbances, which was obtained by using the software package Ipopt/sIpopt.

To demonstrate applicability, a selection of the control structures for the different regions of each case study have been implemented and compared on the dynamic nonlinear models using Simulink.

It has been shown that the first case study, a single distillation column with constant product prices, has 3 active constraint regions while the next, a single distillation column with purity dependent prices, has 5 active constraint regions. The last case study, two distillation columns in sequence with constant prices, has 8 active constraint regions.



# Sammendrag

Undersøking og kartlegging av aktive begrensingsområder for prosesser, for deretter å finne reguleringsstrukturer for hver region, er avgjørende for deres optimale drift. Dette arbeidet tar for seg aktive begrensingsområder for tre forskjellige studier av destillasjon:

- En enkel destillasjonskolonne med faste priser.
- En enkel destillasjonskolonne hvor produktprisen er proporsjonal renheten av produktet.
- To destillasjonskolonner i serie med faste priser.

De aktive begrensingsområdene for hver studie har blitt identifisert og kartlagt med hensyn på forstyrrelsene energipris og fødehastighet. I hvert område har utvalgte trinntemperaturer og kombinasjoner av trinntemperaturer blitt foreslått som selv – optimaliserende variabler for de ubrukte frihetsgradene. Disse ble funnet ved bruk av *Minimum Singular Value Rule* og *Exact Local Method*. For å bruke de to metodene trengs de optimale sensitivitetene til målingene. Dataverktøyet *slpopt* ble brukt til dette.

Noen av de foreslåtte reguleringsstrukturene for de ulike områdene i hver studie har blitt implementert og sammenlignet på de dynamiske ikke – lineære modellene i *Simulink*.

Det har blitt vist at første studie, en enkelt destillasjonskolonne med faste produktpriser, har 3 aktive begrensingsområder. Neste studie, en enkelt destillasjonskolonne hvor produktprisen er proporsjonal renheten av produktet, har 5 aktive begrensingsområder. Den siste studien, to destillasjonskolonner i serie med faste priser, har 8 aktive begrensingsområder.



# Preface

This thesis was written as the final part of my M.sc degree in Chemical engineering at the Norwegian University of Science and Technology.

First, I would like to express my profound gratitude to my supervisors, Post-doc Johannes Jäschke, and Professor Sigurd Skogestad for their invaluable help throughout my work with this thesis.

Thank you both!

Second, I would also like to thank my friends at the Process-systems engineering group for the good companionship. Especially the weekly football sessions have been memorable.

## Declaration of Compliance

I hereby declare that this is an independent work in compliance with the exam regulations of the Norwegian University of Science and Technology.

Trondheim, July 5, 2012

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Roald Bræck Leer





# Contents

<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Problem Description . . . . .	2
<b>2</b>	<b>Background</b>	<b>3</b>
2.1	Distillation . . . . .	3
2.2	Optimization . . . . .	7
2.3	Numerical Tools . . . . .	8
2.3.1	Matlab/Simulink . . . . .	8
2.3.2	Ipopt . . . . .	8
2.3.3	sIpopt . . . . .	8
2.3.4	AMPL . . . . .	8
2.4	Self – optimizing Control . . . . .	9
2.4.1	Minimum Singular Value Rule . . . . .	11
2.4.2	Exact Local Method . . . . .	13
<b>3</b>	<b>Cases</b>	<b>15</b>
3.1	Model . . . . .	16
3.2	Case Study 1a . . . . .	16
3.2.1	Degrees of Freedom . . . . .	17
3.2.2	Disturbances . . . . .	17
3.2.3	Optimization Problem . . . . .	18
3.2.4	Constraints . . . . .	18
3.3	Case Study 1b . . . . .	19
3.3.1	Degrees of Freedom . . . . .	19
3.3.2	Disturbances . . . . .	19
3.3.3	Optimization Problem . . . . .	19
3.3.4	Constraints . . . . .	19
3.4	Case study 2 . . . . .	20
3.4.1	Degrees of Freedom . . . . .	21
3.4.2	Disturbances . . . . .	21
3.4.3	Optimization Problem . . . . .	21
3.4.4	Constraints . . . . .	21

<b>4</b>	<b>Results</b>	<b>23</b>
4.1	Active Constraint Regions . . . . .	23
4.1.1	Case Study 1a . . . . .	23
4.1.2	Case Study 1b . . . . .	24
4.1.3	Case Study 2 . . . . .	25
4.2	Self – optimizing variables . . . . .	28
4.2.1	Minimum Singular Value Rule . . . . .	28
4.2.2	Case Study 1a . . . . .	28
4.2.3	Case Study 1b . . . . .	29
4.2.4	Case Study 2 . . . . .	29
4.2.5	Exact Local Method . . . . .	34
4.3	Simulations . . . . .	35
4.3.1	Case Study 1a . . . . .	35
4.3.2	Case Study 1b . . . . .	36
4.3.3	Case Study 2 . . . . .	37
<b>5</b>	<b>Discussion</b>	<b>39</b>
5.1	Maps of the Active Constraint Regions . . . . .	39
5.1.1	Comparison With Previous Work . . . . .	40
5.2	Minimum Singular Value Rule . . . . .	42
5.3	Simulations . . . . .	43
5.4	Ipopt/sIpopt . . . . .	43
<b>6</b>	<b>Conclusion</b>	<b>45</b>
<b>7</b>	<b>Further Work</b>	<b>47</b>
<b>A</b>	<b>Combinations of temperatures as self – optimizing variables</b>	<b>51</b>
<b>B</b>	<b>Pairing</b>	<b>57</b>
B.1	Case study 1a . . . . .	57
B.2	Case study 1b . . . . .	58
B.3	Case study 2 . . . . .	59
<b>C</b>	<b>Temperature profiles</b>	<b>63</b>
C.1	Case 1a . . . . .	63
C.2	Case 1b . . . . .	64
C.3	Case 2 . . . . .	65
<b>D</b>	<b>AMPL code</b>	<b>69</b>

# Chapter 1

## Introduction

Today, separation of chemical components plays an important part of modern life. Whether it is industrial large scale separation or small scale separation performed in a lab. Separation is defined as as:

*“A process of any scale by which the components of a mixture are separated from each other without substantial chemical modification”* (Cooke & Poole 2000)

The range and scope of the different techniques are numerous to accommodate for all the different separation processes. Distillation is a commonly used separation process in the chemical industry. It is used substantially in the oil and gas sector. E.g. when refined, crude oil is separated by distillation into fractions of naphtha, diesel, gas, jet fuel, etc. With the new boom in the oil industry and an ever present need for fossil fuels, the focus on research and innovation in this area is crucial.

Over the years, distillation has been thoroughly researched and documented. Control of distillation columns is also well investigated in numerous books and articles. However, there has been surprisingly few investigations into optimal operation and active constraints, as pointed out by Jacobsen in his thesis (Jacobsen 2011).

To ensure optimal operation one needs to know how the active constraints change with respect to disturbances. A control structure for one active constraint region may not be feasible for another region where different constraints are active. Locating and mapping these regions provides useful information when choosing control structures.

Selection of good controlled variables and implementing these in a control structure plays an important part of optimal operation. The term *“good controlled variables”* reflects the basis for the idea of self – optimizing control (Skogestad 2000). Finding and controlling some key variables to a constant value so that the process runs close to an optimum.

These variables may be found by applying different methods, like the Minimum Singular Value Rule (Skogestad & Postletwaite 1996) and the Exact Local Method (Halvorsen, Skogestad, Morud & Alstad 2003) to a set of measurements.

This work is twofold. Locating and mapping the active constraint regions for the different case studies, and proposing self – optimizing control structures for each region. Also, the software package *Ipopt/sIpopt* (Wächter & Biegler 2006) is used in this work to test it on a self – optimizing control study.

## 1.1 Problem Description

This assignment continues on Magnus Jacobsen’s work of identifying active constraint regions for optimal operation of distillation columns.

In his thesis Jacobsen examines the active constraint regions for three cases:

1. A single distillation column with constant product prices.
2. A single distillation column with purity dependent product prices.
3. Two distillation columns in sequence with constant prices.

Although identifying these regions, Jacobsen did not pursue finding the self – optimizing variables for the unconstrained degrees of freedom. The purpose of this work is to find self – optimizing control structures for each of the active constraint regions previously found by Jacobsen. The idea is that by keeping certain variables or combinations of variables constant, the distillation column will operate close to the optimum without having to re-optimize for disturbances.

Mapping the active constraint regions for each of the cases will be redone to allow for comparison of previous work. A steady – state distillation model will be written in the in the mathematical programming language AMPL (Fourer, Gay & Kerningham 2003) and optimized using the open software *Ipopt/sIpopt* (Wächter & Biegler 2006). The model is based on the distillation Column A (Morari & Skogestad 1988).

In each of the active constraint regions the model will be linearized to find candidates for the self – optimizing controlled variables. The Minimum Singular Value Rule and the Exact Local Method will be used to find these. Selected self – optimizing control structures will then be compared and tested on the dynamic nonlinear models using Matlab/Simulink.

# Chapter 2

## Background

In this chapter relevant theory for the thesis will be introduced. The process of distillation is presented and pertinent equations derived. Relevant optimization theory is gone through along with brief introductions of the tools used. The principle behind self – optimizing control is explained as well as the methods for finding self – optimizing variables.

### 2.1 Distillation

Distillation is one of the most important separation technologies in the industry. It may be described as a countercurrent multistage flash. If you increase the number of equilibrium stages almost any degree of separation, with a fixed energy consumption, is possible (Halvorsen & Skogestad 2000). This makes distillation particularly good for high purity separations. A simple schematic of a distillation stage is shown in Figure 2.1. Liquid is flowing downwards through the column, entering the stage from the top. It is mixed with the vapor flowing upwards and equilibrium is reached. This is distillation stage concept. At each theoretical stage one assumes that vapor – liquid equilibrium(VLE) is reached. This may not be true for all columns, i.e. packed columns, but it has been established that the concept fits well with experimental data from real columns (Halvorsen & Skogestad 2000).

For a two – component system, with  $N_c$  non reacting components, the state is determined by  $N_c$  degrees of freedom. The degrees of freedom,  $f$ , is given from Gibb's phase rule:

$$f = N_c + 2 - ph \tag{2.1}$$

Here  $ph$  is the number of phases. Setting the pressure,  $P$ , and the liquid mole fractions,  $x$ , as degrees of freedom, the temperature,  $T$ , and the vapor mole fractions,  $y$ , are determined. The VLE then is written:

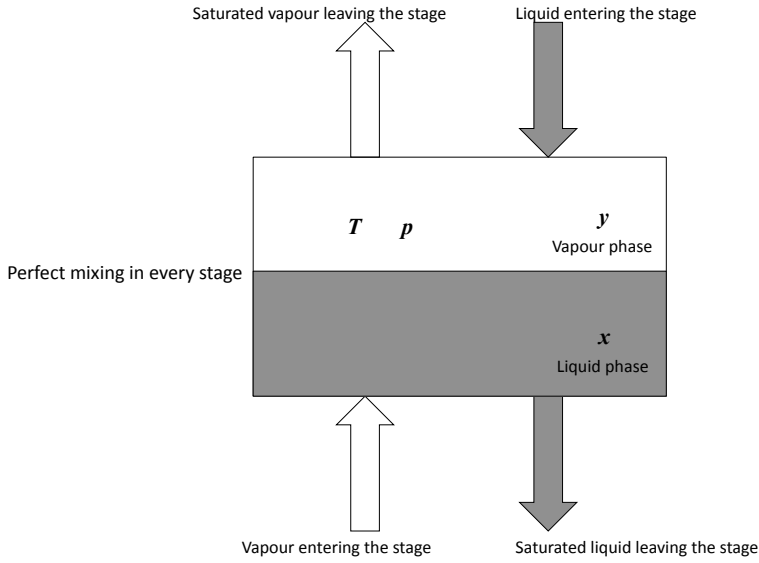


Figure 2.1: Equilibrium – stage concept.

$$\begin{aligned} [y_1, y_2 \cdots, y_{N_c-1}] &= f(P, x_1, x_2 \cdots, x_{N_c-1}) \\ [y, T] &= f(P, x) \end{aligned} \quad (2.2)$$

The mole fractions in the liquid phase  $\sum_{i=1}^n x_i = 1$  and in the vapor phase  $\sum_{i=1}^n y_i = 1$ , where  $n$  is the number of stages. The familiar Raoult's law states that for ideal mixtures the partial pressure of a component in the vapor phase is proportional to the partial pressure of the pure component  $p_i = x_i p_i^\circ(T)$ . Dalton's law for ideal gases states that the partial pressure of a component is proportional to the mole fraction  $p_i = y_i P$ . Combining these two equations, and adding that the total pressure of the system is a combination of the partial pressures, one can derive the following relationship:

$$y_i = x_i \frac{p_i^\circ}{P} = \frac{x_i p_i^\circ(T)}{\sum_i x_i p_i^\circ(T)} \quad (2.3)$$

For a component  $i$ , the K – value is defined as follows:

$$K_i = \frac{y_i}{x_i} \quad (2.4)$$

From the  $K$  – values the relative volatility is derived, which is a measure of comparing the vapor pressures of the components in a liquid mixture. It is desirable to have a large relative volatility when separating two components due to the implication that there is a large difference between the boiling points of the components, making the separation easier. Applying Raoult’s law for ideal mixtures, the relative volatility becomes:

$$\alpha_{ij} = \frac{(y_i/x_i)}{(y_j/x_j)} = \frac{K_i}{K_j} = \frac{p_i^\circ(T)}{p_j^\circ(T)} \quad (2.5)$$

The partial pressure is dependent on the temperature and thus the  $K$  – values are dependent on temperature. Combining Equations (2.3) and (2.5) gives the VLE – relationship. For a binary mixture this is:

$$y_i = \frac{\alpha_i x_i}{\sum_i \alpha_i x_i} \quad (2.6)$$

Removing the indices for the light component and setting  $x = x_1$  and  $x_2 = 1 - x$  Equation (2.6) becomes:

$$y = \frac{\alpha x}{1 + (\alpha - 1)x} \quad (2.7)$$

### Ternary Mixtures

Equation (2.3) can be used for ternary mixtures (Stichlmair & Fair 2000). Given the three components  $A$ ,  $B$  and  $C$ , where  $A$  is the light component,  $B$  is the middle one and  $C$  the heavy, the VLE – relationship for component  $A$  is:

$$y_A = \frac{x_A p_A^\circ}{x_A p_A^\circ + x_B p_B^\circ + x_C p_C^\circ} \quad (2.8)$$

The relative volatilities are  $\alpha_{AC} = p_A^\circ/p_C^\circ$ ,  $\alpha_{BC} = p_B^\circ/p_C^\circ$  and  $\alpha_{AB} = p_A^\circ/p_B^\circ$ . Substituting the relative volatilities into the Equation (2.8) and setting  $x_C = 1 - x_A - x_B$  gives:

$$y_A = \frac{x_A \alpha_{AC}}{1 + (\alpha_{AC} - 1)x_A + (\alpha_{BC} - 1)x_B} \quad (2.9)$$

### Material Balance

The distillation column is modeled as a series of connected stages, as seen in Figure 2.2. Each stage is in equilibrium, and perfect mixing is assumed in each phase.

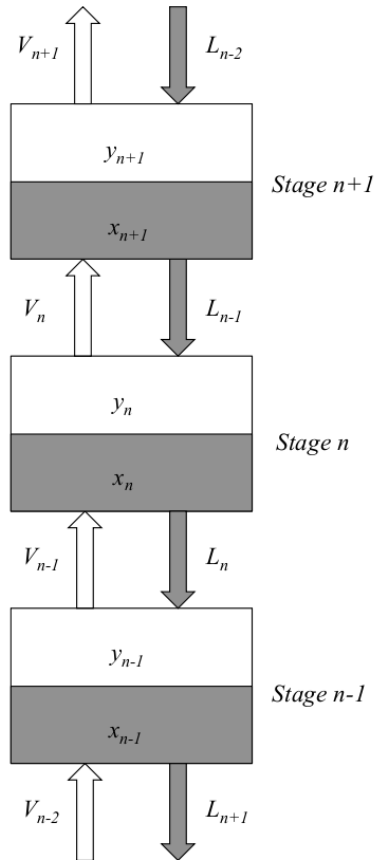


Figure 2.2: Distillation column modeled as a set of connected equilibrium stages.



Based on Figure 2.2 the material balance for component  $i$  at stage  $n$  is:

$$\frac{dN_{i,n}}{dt} = (L_{n-1}x_{i,n-1} - V_n y_{i,n}) - (L_n x_{i,n} - V_{n-1} y_{i,n-1}) \quad (2.10)$$

Here  $N_{i,n}$  is the number of moles of component  $i$  at stage  $n$ .  $L$  and  $V$  are the liquid and vapor flow rates. The net material flow,  $w_i$ , is defined as:

$$w_{i,n} = V_n y_{i,n} - L_{n+1} x_{n+1} \quad (2.11)$$

For steady – state operation the change  $N_{i,n}$  is zero,  $\frac{dN_{i,n}}{dt} = 0$ . Also, the net material flow is constant through the column at steady – state. Equation (2.11) can be rewritten as the equation for the Operating line:

$$y_{i,n} = \frac{L_{n+1}}{V_n} x_{i,n} + \frac{1}{V_n} w_i \quad (2.12)$$

This, together with the VLE – relation, makes it possible to compute all the stage compositions for the system.

## 2.2 Optimization

A nonlinear minimization problem is defined as:

$$\begin{aligned} \min_x \quad & J(x, u, d) \\ \text{subject to} \quad & c_i(x, u, d) = 0 \quad i \in \mathcal{E} \\ & c_i(x, u, d) \leq 0 \quad i \in \mathcal{I} \end{aligned} \quad (2.13)$$

$J$  is the cost function, the index set  $\mathcal{E}$  denotes the equations which are equality constraints (the process model) and the set  $\mathcal{I}$  denotes the indices of the inequality constraints.  $x$  are the internal variables,  $u$  are the manipulated variables and  $d$  are the disturbances.

For a minimization problem as given in Equation (2.13) a cost function is minimized over the expected disturbances while satisfying the process constraints (Jacobsen 2011). After formulating a model, an optimization algorithm is used to find a solution. When the solution is found it may be checked by using optimality conditions.

Lagrange multipliers,  $\lambda$ , are introduced as a tool for finding a solution to the optimization problem. By defining a new function,  $\mathcal{L}$ , and using  $\lambda$ , the optimization problem becomes:

$$\mathcal{L} = J(x, u, d) - \lambda c_i(x, u, d) \quad (2.14)$$

The solution is characterized by the The Karush – Kuhn – Tucker conditions (abbreviated KKT – conditions), which are necessary for a first-order solution to be optimal (Nocedal & Wright 1999). The KKT – conditions are defined:

$$\begin{aligned}
 \nabla_x \mathcal{L}(x^*, u^*, \lambda^*) &= 0 \\
 c_i(x^*, u^*) &= 0 \quad \text{for all } i \in \mathcal{E}, \\
 c_i(x^*, u^*) &\geq 0 \quad \text{for all } i \in \mathcal{I}, \\
 \lambda_i^* &\geq 0 \quad \text{for all } i \in \mathcal{I}, \\
 \lambda_i^* c_i(x^*, u^*) &= 0 \quad \text{for all } i \in \mathcal{E} \cup \mathcal{I},
 \end{aligned} \tag{2.15}$$

$x^*$ ,  $u^*$  and  $\lambda^*$  are the notations for the variables at the optimal solution.

## 2.3 Numerical Tools

The different tools used in this work are presented in this section.

### 2.3.1 Matlab/Simulink

Simulink is an environment in Matlab, used for multidomain simulation and model – based design for dynamic and embedded systems (MathWorks 2012).

### 2.3.2 Ipopt

The open source software package IPOPT (Interior point optimizer) is an optimization software for large – scale nonlinear optimization problems. The algorithm is a primal – dual interior point algorithm with a filter line search (Wächter & Biegler 2006).

### 2.3.3 sIpopt

Optimal Sensitivity Based on Ipopt is a toolbox for Ipopt. This toolbox allow the user to change parameters of the optimization problem to generate fast solutions (*sIpopt Documentation* 2012).

### 2.3.4 AMPL

AMPL – “*a mathematical programming language*” is a modeling language for solving mathematical problems, typically optimization problems. It was developed and designed by Robert Fourer, David M. Gay and Brian W. Kernigham around 1985 (Fourer et al. 2003).

An advantage with the syntax of AMPL is its similarity to normal mathematical notation. This thesis uses AMPL as the interface for the solvers Ipopt and

sIpopt.

## 2.4 Self – optimizing Control

Optimal operation of chemical plants requires a control structure that drives the economic profit to a maximum under varying operating conditions while maintaining acceptable operation (Skogestad 2000). According to the time scale in which they operate, the control system is usually divided into a hierarchy of several layers where the set points of the controlled variables,  $c_s$ , are the internal variables that link the layers together. This is shown in Figure 2.3. The layers include scheduling(weeks), site – wide optimization(days), local optimization(hour), supervisory control(minutes) and regulatory control(seconds). The hierarchy functions so that the upper layers compute the set points for the layers below.

As previously mentioned, one always wants a system to operate as close to the optimum as possible. Maximizing the profits is equivalent to minimizing a scalar cost function. The cost function,  $J$ , defines the cost for operation. A simple strategy to solve this kind of problem is to somehow get the system to self-optimize for different disturbances, instead of doing online optimization for every one. This is the idea behind *Self – optimizing control*.

Skogestad gives the following definition for self – optimizing control (Skogestad 2000):

*“Self – optimizing control is when we can achieve an acceptable loss with constant set point values for the controlled variables (without the need to reoptimize when disturbances occur).“*

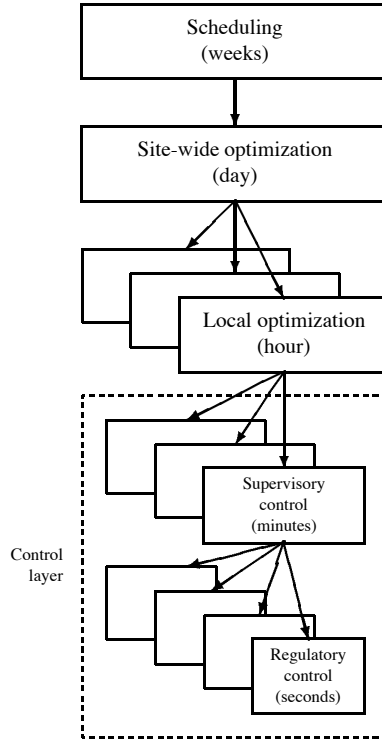


Figure 2.3: Typical control hierarchy for a chemical plant (Skogestad & Postlethwaite 2005).

So, the key to deciding a self – optimizing control structure is to find what these internal variables should be.

The loss is defined from the previously mentioned cost function as the difference between actual operating costs for the controlled system and the optimal operational costs:

$$L(u, d) = J(u, d) - J_{opt}(d) \quad (2.16)$$

$L$  is the loss,  $J$  is the actual costs and  $J_{opt}$  is the actual costs at the optimum. As seen in Equation (2.16), a small difference between  $J$  and  $J_{opt}$  is obviously wanted. This is done in practice by using the degrees of freedom for the system to control the optimal active constraints and using the remaining degrees of freedom to keep the self – optimizing variables at a constant setpoint. This method will generally impose some loss compared to reoptimization for every disturbance. The aim is to choose the right variables to control so that the loss is small and acceptable. Figure 2.4 illustrates this. Using  $c_1$  as a self – optimizing variable results in a smaller loss

than selecting  $c_2$  as a self – optimizing variable.

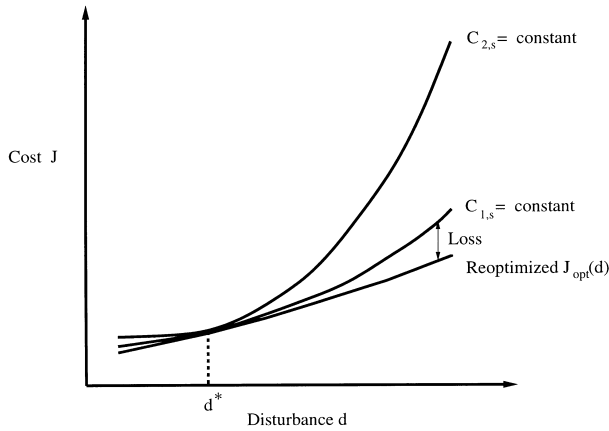


Figure 2.4: Loss imposed by keeping constant set point for the controlled variable (Skogestad & Postlethwaite 2005).

Different strategies are employed to select good controlled variables. Intuitively, a controlled variable needs to be insensitive to disturbances at its optimal point so that the optimum does not shift for disturbances. Also, the optimum should be flat and therefore avoid problems with implementation errors. 4 requirements for a "good" controllable variables are given in (Skogestad 2000):

- *Requirement 1:* Its optimal value should be insensitive to disturbances.
- *Requirement 2:* It should be easy to measure and control accurately.
- *Requirement 3:* Its value should be sensitive to changes in the manipulated variables.
- *Requirement 4:* For cases with two or more controllable variables, the selected variables should not be too closely correlated.

Two methods are used in this work to find these variables: The Minimum Singular Value Rule (Skogestad & Postlethwaite 1996) and the Exact Local Method (Halvorsen et al. 2003).

### 2.4.1 Minimum Singular Value Rule

As mentioned previously the remaining degrees of freedom, after the active constraints are handled, are used to keep the controlled variables at constant set points.

For small deviations around the optimal point it is possible to use a linear relationship between the degrees of freedom,  $u$ , and the candidate set of controlled variables,  $c$ :

$$\Delta c = G\Delta u + G_d\Delta d \quad (2.17)$$

Here,  $\Delta u = u - u_{opt}$  and  $\Delta c = c - c_{opt}$ .  $G$  is the steady – state gain matrix, and  $G_d$  the disturbance model. If the disturbances are fixed and  $G$  is invertible:

$$u - u_{opt} = G^{-1}(c - c_{opt}) \quad (2.18)$$

Expressing the cost function in terms of a Taylor expansion around the optimal point with fixed disturbances results in:

$$\begin{aligned} J(u, d) = & J_{opt}(d) + \left( \frac{\partial J}{\partial u} \right)_{opt}^T (u - u_{opt}(d)) \\ & + \frac{1}{2} (u - u_{opt}(d))^T \left( \frac{\partial^2 J}{\partial u^2} \right)_{opt} (u - u_{opt}(d)) + \dots \end{aligned} \quad (2.19)$$

The higher orders terms are neglected. Notice that the term  $\left( \frac{\partial J}{\partial u} \right)_{opt}^T = 0$  at the optimum for an unconstrained problem. Equation (2.16) can now be rewritten with the second – order expansion,

$$L = J(u, d) - J(u_{opt}(d), d) \approx \frac{1}{2} (u - u_{opt}(d))^T J_{uu} (u - u_{opt}(d)) \quad (2.20)$$

where  $J_{uu} = \left( \frac{\partial^2 J}{\partial u^2} \right)_{opt}$ . By using Equation (2.18), and introducing  $z = J_{uu}^{1/2} G^{-1}(c - c_{opt})$ , the equation simplifies:

$$L = \frac{1}{2} \|z\|_2^2 \quad (2.21)$$

The notation  $\|z\|_2$  denotes the 2 – norm of the expression. Each controlled variable,  $c_i$ , is assumed to be scaled so that the sum of its optimal range,  $v_i$ , and its implementation error,  $n_i$ , is unity. The combined errors of the 2 – norm is less than 1. The inputs,  $u$ , are scaled so that they have the same effect on the cost. This gives a worst – case loss:

$$\max_{\|c - c_{opt}\|_2 \leq 1} L = \frac{1}{2} \bar{\sigma}^2 (\alpha^{1/2} G^{-1}) = \frac{\alpha}{2} \frac{1}{\bar{\sigma}(G)} \quad (2.22)$$

The constant  $\alpha = \bar{\sigma}$  is independent of the choice of controlled variables.  $\bar{\sigma}$  denotes the minimum singular value. Equation (2.22) then states that one should choose controlled variables that maximizes the minimum singular value of the scaled gain matrix  $G$ , from  $u$  to  $c$  (Skogestad & Postletwaite 1996), (Halvorsen et al. 2003).

### 2.4.2 Exact Local Method

The Exact Local Method was derived from the Exact Method based on ‘brute force’ evaluation (Halvorsen et al. 2003). From Halvorsen et al. (2003)  $z$  can be written,

$$z = J_{uu}^{1/2}[(J_{uu}^{-1}J_{ud} - G^{-1}G_d)(d - d_{opt}) + G^{-1}n] \quad (2.23)$$

where  $n$  is the implementation error. Notice that the term  $J_{ud} = \left(\frac{\partial^2 J}{\partial u \partial d}\right)_{opt}$ . Two positive diagonal matrices,  $W_d$ , and  $W_n^y$  are introduced.  $W_d$  represents the expected magnitudes of the individual disturbances.  $W_n^y$  represents the magnitude of the implementation error for each candidate measurement  $y$ . The controlled variables are a function of the candidate measurements and can linearly be written as follows:

$$\Delta c = H\Delta y \quad (2.24)$$

$H$  is the measurement combination matrix. The expected magnitudes of the disturbances can be written:

$$d - d_{opt} = W_d d' \quad (2.25)$$

The disturbance is normalized so that  $y' < 1$ . The implementation error is:

$$n = HW_n^y n^{y'} = W_n n^{y'} \quad (2.26)$$

Also  $n^{y'}$  is normalized to have a value of less than 1. More precisely, the combined disturbances and implementation errors are 2 – norm – bounded:

$$\|f'\|_2 \leq 1; f' \triangleq \begin{pmatrix} d' \\ n^{y'} \end{pmatrix} \quad (2.27)$$

Then the worst – case loss can be formulated as (Halvorsen et al. 2003) :

$$\max_{\|f'\|_2 \leq 1} L = \bar{\sigma}(M)^2/2 \quad (2.28)$$

where

$$M = (M_d \ M_n) \quad (2.29)$$

$$M_d = J_{uu}^{1/2}(HG^y)^{-1}HFW_d \quad (2.30)$$

$$M_n = J_{uu}^{1/2}(HG_d^y)^{-1}HW_n^y \quad (2.31)$$

where  $F = \frac{\partial y^{opt}}{\partial d}$  is the sensitivity matrix. The average loss (Kariwala, Cao & Janardhanan 2008) is defined:

$$L = \frac{1}{2}\|M\|_F^2 \quad (2.32)$$

To find the  $H$  – matrix that minimize the worst – case loss and average loss, the Minimum loss method is introduced (Alstad, Skogestad & Hori 2009), where  $H$  is selected to minimize,

$$\min_H \|J_{uu}^{1/2}(HG^y)^{-1}HY\|_F \quad (2.33)$$

Here,  $Y = [FW_d \ W_n^y]$ . The  $H$  – matrix which minimizes Equation (2.33) is found by:

$$H = G^{yT}(YY^T)^{-1} \quad (2.34)$$

This minimizes both the average loss and worst – case loss (Kariwala et al. 2008).



# Chapter 3

## Cases

Based on the thesis of Jacobsen (2011), three different case studies were investigated in this work:

- **Case study 1a:** One distillation column with constant product prices.
- **Case study 1b:** One distillation column with purity dependent prices.
- **Case study 2:** Two distillation columns in sequence with constant product prices.

For each case study the active constraint regions will be identified, drawn and compared to previous results (Jacobsen 2011). Each region with unconstrained degrees of freedom will be further investigated to find self – optimizing variables for control. It is assumed that only temperatures and concentrations at the top and bottom streams are available for control. The Minimum Singular Value rule and the Exact Local Method is used for this purpose. A selection of the self – optimizing control structures were tested using dynamic simulation of the different cases.

The component system were chosen to be:

- **Case 1a,b:** Toulene and benzene
- **Case 2:** Toluene, benzene and p – xylene

The temperatures for the binary distillation cases were assumed to depend linearly on liquid composition (Hori & Skogestad 2007),

$$T_i = T_{B,H}x_i^H + T_{B,L}x_i^L \quad (3.1)$$

where  $T_{B,H}$  is the boiling temperature for the heavy component,  $x_i^H$  the mole fraction of heavy component,  $T_{B,L}$  is the boiling point for the light component and  $x_i^L$  is the mole fraction of the light component.

For ternary distillation the relation is assumed to be:

$$T_i = T_{B,H}x_i^H + T_{B,M}x_i^M + T_{B,L}x_i^L \quad (3.2)$$

Here  $T_{B,M}$  is the boiling temperature for middle component and  $x_i^M$  is its mole fraction.

### 3.1 Model

The basis for the case studies is the steady – state model *Column A* (Morari & Skogestad 1988), with  $L/V$  configuration. It has been written in AMPL. The assumptions for the model are listed in Table 3.1.

Table 3.1: Assumptions for *Column A*.

Assumptions	
1	Constant pressure
2	Constant relative volatility
3	Equilibrium on all stage
4	Total condenser
5	Constant molar flows
6	No vapor holdup
7	Linearized liquid dynamics
8	Effect of vapor flow on liquid flow

### 3.2 Case Study 1a

The first case study is a single distillation column with constant product prices. The column has 41 stages including reboiler where the feed enters at stage 21. The feed consists of components A and B, where A is the light component and B is the heavy. Figure 3.1 shows an illustration of a distillation column.

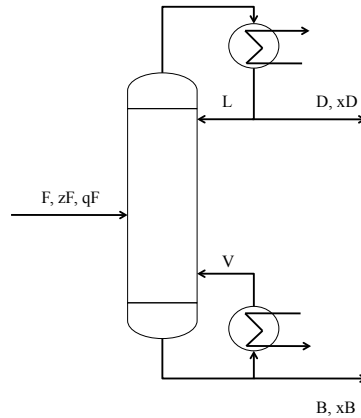


Figure 3.1: Illustration of a single distillation column.

### 3.2.1 Degrees of Freedom

Assuming that both the pressure and the feed are given, the distillation column has two steady – state degrees of freedom (Skogestad, Lundström & Jacobsen 1990). There are dynamically four manipulated variables. Two of the four have been selected to control the levels in the condenser and the reboiler. They have no steady – state effect. The two degrees of freedom are then selected as the reflux and boilup in the column:

$$u = [L, V] \quad (3.3)$$

### 3.2.2 Disturbances

There are several disturbances for a distillation process. In this case study, as well as the other two, only the feed flow rate and energy price are used as disturbances when mapping the active constraint regions. The intention is to get a good graphical presentation of the regions.

$$d = [F, p_V] \quad (3.4)$$

Note that when finding the self – optimizing variables, the feed liquid fraction,  $qF$ , and feed composition,  $zF$ , are also included as disturbances.

### 3.2.3 Optimization Problem

The optimization problem for case 1a is formulated:

$$\begin{aligned}
 \min_u \quad & J(u, d) = p_F F + p_V V - p_B B - p_D D \\
 \text{subject to} \quad & x_B \geq x_{B,min} \\
 & x_D \geq x_{D,min} \\
 & V \leq V_{max}
 \end{aligned} \tag{3.5}$$

The  $p$  – values are the prices for the different flows. The inputs  $u = [L, V]$  and the disturbances  $d = [F, p_V]$ .

### 3.2.4 Constraints

The constraints for a single column with constant prices are purity specific constraints and capacity constraints:

1. The mole fraction of light component in the distillate should be equal or larger than a minimum value,  $x_D \geq x_{D,min}$ .
2. The mole fraction of heavy component in the bottom should be equal or larger than a minimum value,  $x_B \geq x_{B,min}$ .
3. The boilup should be less or equal to a maximum value,  $V \leq V_{max}$ .

Key data needed for the case studies 1a and 1b are given in Table 3.2, The values used were taken from Jacobsen (2011).

Table 3.2: Key data for case study 1a and 1b.

Variables	Value
$\alpha_{AB}$	1.5
$z_F$	0.5
$F$	0 – 1.6 kmol/min
$qF$	1
$p_F$	\$ 1
$p_V$	\$ 0 – 0.02
$p_D$	\$ 2
$P_B$	\$ 1
$x_{D,min}$	0.95
$x_{B,min}$	0.99
$V_{max}$	4.008 kmol/min

### 3.3 Case Study 1b

Case study 1b is similar to the first. However, now the price of distillate,  $p'_D$ , is proportional to the purity:

$$p'_D = p_D x_D \quad (3.6)$$

The reason for using a variable distillate price is to simulate a case where energy is cheap. With a low energy price it is possible to overpurify the distillate as the price is proportional to the purity.

#### 3.3.1 Degrees of Freedom

The two degrees of freedom are the same the previous case, reflux and boilup in the column:

$$u = [L, V] \quad (3.7)$$

#### 3.3.2 Disturbances

The disturbances are:

$$d = [F, pV] \quad (3.8)$$

#### 3.3.3 Optimization Problem

This gives the following optimization problem for case 1b:

$$\begin{aligned} \min_u \quad & J(u, d) = p_F F + p_V V - p_B B - p'_D D \\ \text{subject to} \quad & x_B \geq x_{B, \min} \\ & x_D \geq x_{D, \min} \\ & V \leq V_{\max} \end{aligned} \quad (3.9)$$

#### 3.3.4 Constraints

The constraints are the same as for case study 1a:

1. The mole fraction of light component in the distillate should be equal or larger than a minimum value,  $x_D \geq x_{D, \min}$ .
2. The mole fraction of the heavy component in the bottom should be equal or larger than a minimum value,  $x_B \geq x_{B, \min}$ .
3. The boilup should be less or equal to a maximum value,  $V \leq V_{\max}$ .

### 3.4 Case study 2

The model for case study 2 consists of two distillation columns in sequence with a ternary component system. The three components are A, B and C, where A is the lightest component, B is the middle one and C is the heavy component. B is the most valuable product. All prices are constant for case study 2. Figure 3.2 shows an illustration of two columns in sequence. The two columns have 41 stages each, with the feed entering column 1 at stage 21, and the bottom product from column 1 enters column 2 at stage 1.

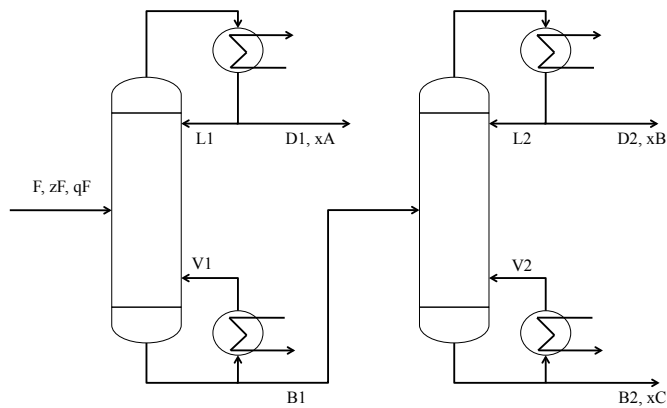


Figure 3.2: Illustration of two distillation columns in sequence.

### 3.4.1 Degrees of Freedom

For the ternary system the distillation column has four steady – state degrees of freedom. Similar to the previous cases the liquid levels in the condensers and reboilers are controlled, claiming four out of the eight dynamic manipulated variables. Again, they have no steady – state effect. The remaining four degrees of freedom are selected as:

$$u = [L1, V1, L2, V2] \quad (3.10)$$

Here,  $L1$  and  $V1$  are the reflux and boilup for column 1, while  $L2$  and  $V2$  are the reflux and boilup for column 2.

### 3.4.2 Disturbances

The disturbances are:

$$d = [F, pV] \quad (3.11)$$

### 3.4.3 Optimization Problem

$$\begin{aligned} \min_u \quad & J(u, d) = p_F F + p_V (V1 + V2) - p_A D1 - p_B D2 - p_C B2 \\ \text{subject to} \quad & x_A \geq x_{A,min} \\ & x_B \geq x_{B,min} \\ & x_C \geq x_{C,min} \\ & V1 \leq V1_{max} \\ & V2 \leq V2_{max} \end{aligned} \quad (3.12)$$

### 3.4.4 Constraints

The constraints for the ternary system is:

1. The mole fraction of component A in the distillate of column 1 should be equal or larger than a minimum value,  $x_A \geq x_{A,min}$ .
2. The mole fraction of component B in the distillate of column 2 should be equal or larger than a minimum value,  $x_B \geq x_{B,min}$ .
3. The mole fraction of component C in the bottom of column 2 should be equal or larger than a minimum value,  $x_C \geq x_{C,min}$ .

4. The boilup of column 1 should be less or equal to a maximum value,  $V1 \leq V1_{max}$ .
5. The boilup of column 2 should be less or equal to a maximum value,  $V2 \leq V2_{max}$ .

Key data used in optimization of case study 2 are given in Table 3.3.

Table 3.3: Key data for case study 2.

Variables	Value
$\alpha_{AB}$	1.33
$\alpha_{BC}$	1.5
$\alpha_{AC}$	1.0
$z_F$	[0.4 0.2 0.4]
$F$	0 – 1.6 kmol/min
$qF$	1
$p_F$	\$ 1
$p_V$	\$ 0 – 0.02
$p_A$	\$ 1
$P_B$	\$ 2
$P_C$	\$ 1
$x_{A,min}$	0.95
$x_{B,min}$	0.95
$x_{C,min}$	0.95
$V1_{max}$	4.008 kmol/min
$V2_{max}$	2.405 kmol/min



# Chapter 4

## Results

In this chapter the results will be presented. First the maps of the active constraint regions. Second, the results from the Minimum Singular Value Rule and the Exact Local Method. And last, the testing of a selection of the proposed self – optimizing control structures on the dynamic nonlinear models.

### 4.1 Active Constraint Regions

For all three case studies, a map of the active constraint regions have been drawn with regard to the disturbances; feed flow rate and energy prices.

#### 4.1.1 Case Study 1a

In case study 1a, a single distillation column with constant prices, three different active constraint regions were found. These regions are sketched in Figure 4.1 and explained in the bullet points.

- **Region I:** Only the mole fraction of component A in the distillate,  $x_D$ , is at its active constraint value. One self – optimizing variable is needed.
- **Region II:** Both the mole fractions of component A in the distillate,  $x_D$ , and component B in the bottom,  $x_B$ , are at their active constraints values. No self – optimizing variables are needed.
- **Region III:** Both the mole fraction of component A in the distillate,  $x_D$ , and the boilup,  $V$ , are at their respective active constraint values. No self – optimizing variables are needed.

Selected values for each of the regions in Figure 4.1 are presented in Table 4.1. The highlighted values represent variables at their active constraint values. It is worth mentioning that in every region the mole fraction of component A in the distillate,  $x_D$ , is at its active constraint value.

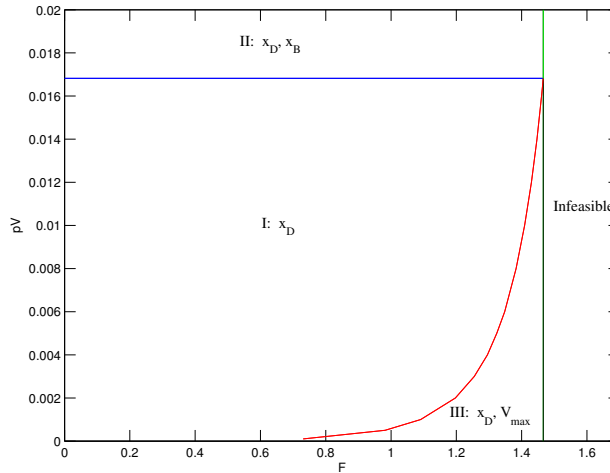


Figure 4.1: Map of the active constraint regions for a single distillation column with constant prices.

#### 4.1.2 Case Study 1b

Case study 1b, a single distillation column with purity dependent prices, gives five active constant regions. These regions are sketched in Figure 4.2. The different regions are explained in the bullet points.

- **Region I:** Only the mole fraction of component B in the bottom,  $x_B$ , is at its active constraint value. One self – optimizing variable is needed.
- **Region II:** Both the mole fractions of component A in the distillate,  $x_D$ , and component B in the bottom,  $x_B$ , are at their respective active constraints values. No self – optimizing variables are need.
- **Region III:** The mole fraction of component B in the distillate,  $x_B$ , and the boilup,  $V$ , are at their active constraint values. No self – optimizing variables are need.
- **Region IV:** The boilup,  $V$ , is at its active constraint value. One self – optimizing variable is needed.
- **Region V:** There are no active constraints. Two self – optimizing variables are needed.

A selection of optimal values for each region are shown in Table 4.2.

Table 4.1: Selection of optimal values for a single column constant product prices.

Region	I	II	III
Feed, $F$	1.2	0.7	1.4
price vapor, $pV$	0.012	0.018	0.002
Liquid flow rate, $LT$	2.7364	1.3275	3.2760
Vapor flow rate, $VB$	3.3631	1.6402	<b>4.008</b>
Distillate, $D$	0.6267	0.3128	0.7320
Bottom, $B$	0.5733	0.2872	0.6680
Fraction of light comp in distillate, $x_D$	<b>0.95</b>	<b>0.95</b>	<b>0.95</b>
Fraction of heavy comp in bottoms, $x_B$	0.9912	<b>0.99</b>	0.9931

Table 4.2: Selection of optimal values for one column with purity dependent prices.

Region	I	II	III	IV	V
Feed, $F$	0.7	0.8	1.4	1.2	0.4
Price vapor, $pV$	0.07	0.12	0.02	0.005	0.01
Price distillate, $pD$	1.9337	1.9000	1.9407	1.9821	1.9823
Liquid flow rate, $LT$	1.6257	1.7700	3.2937	3.4073	1.1402
Vapor flow rate, $VB$	1.9842	2.1870	<b>4.008</b>	<b>4.008</b>	1.3404
Distillate, $D$	0.3585	0.4170	0.7143	0.6007	0.2002
Bottom, $B$	0.3415	0.3830	0.6857	0.5993	0.1998
Fraction of light comp in distillate, $x_D$	0.9668	<b>0.95</b>	0.9704	0.9911	0.9912
Fraction of heavy comp in bottoms, $x_B$	<b>0.99</b>	<b>0.99</b>	<b>0.99</b>	0.9922	0.9923

### 4.1.3 Case Study 2

For the two distillation columns in sequence there are a total of eight active constraints regions. The regions are sketched in Figure 4.3 and explained in the bullet points.

- **Region I:** Only the mole fraction of component B in the distillate of the second column,  $x_B$ , is at its active constraint value. Three self – optimizing variables are needed.
- **Region II:** Both the mole fractions of component A in the distillate of column 1,  $x_A$ , and component B in the distillate of column 2,  $x_B$ , are at their active constraint values. Two self – optimizing variables are needed.

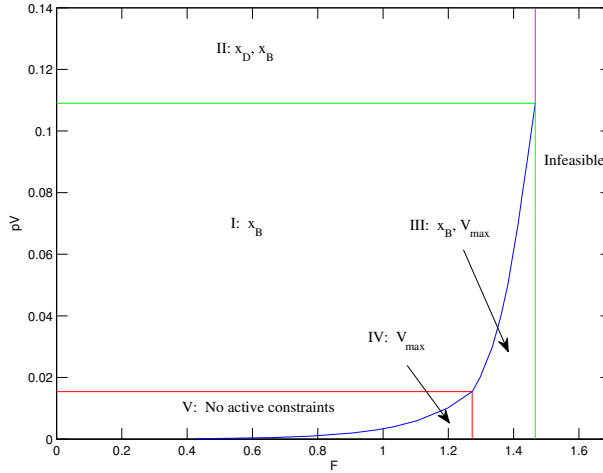


Figure 4.2: Active constraint regions for a single distillation column with purity dependent prices.

- **Region III:** The mole fractions of all three components are at their respective active constraint values. One self – optimizing variable is needed.
- **Region IV:** The mole fraction of component B in the distillate of column 2,  $x_B$ , as well as the boilup for column 1,  $V_1$ , are at their active constraint values. Two self – optimizing variables are needed.
- **Region V:** The two mole fractions of component A in the distillate of column 1,  $x_A$ , and component B in the distillate of column 2,  $x_B$ , and also the boilup of column 1,  $V_1$ , are at their active constraint values. One self – optimizing variables is needed.
- **Region VI:** All component mole fractions are at their respective active constraint values along with the boilup of column 1,  $V_1$ . No self – optimizing variables are needed.
- **Region VII:** The constraint for the mole fraction of component B in the distillate of column 2,  $x_B$ , and both the boilup,  $V_1$  and  $V_2$ , are active. One self – optimizing variable is needed.
- **Region VIII:** The constraints for the mole fractions of component A in column 1,  $x_A$ , and component B in the distillate of column 2,  $x_B$  are active. The boilups of column 1 and column 2,  $V_1$  and  $V_2$ , are also active. No self – optimizing variables are needed.

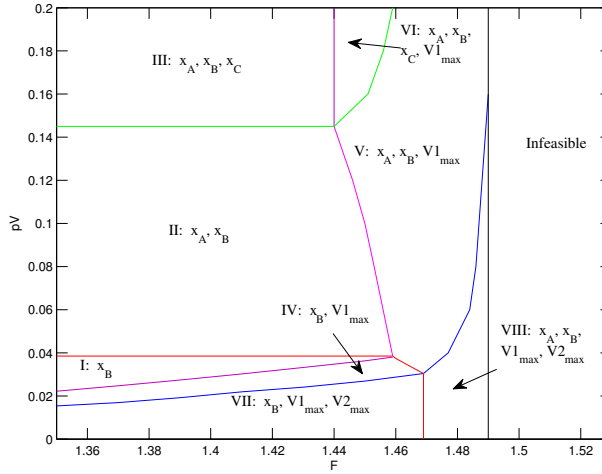


Figure 4.3: Map of the active constraint regions for two columns in sequence with constant prices.

In Table 4.3 selected values for the active constraint regions of case study 2 are shown. Also in this case study there is one constraint,  $x_B$ , which is active for all the regions.

Table 4.3: Selection of optimal values for two columns in sequence with constant prices.

Region	I	II	III	IV	V	VI	VII	VIII
$F$	1.36	1.4	1.4	1.36	1.47	1.45	1.46	1.48
$pV$	0.03	0.09	0.16	0.02	0.1	0.2	0.01	0.02
$LT1$	3.3240	3.2860	3.3122	3.4556	3.4001	3.4075	3.4054	3.3965
$LT2$	1.9668	1.7940	1.6777	2.0809	1.9593	1.7642	2.1365	2.1367
$VB1$	3.8810	3.8657	3.89234	<b>4.008</b>	<b>4.008</b>	<b>4.008</b>	<b>4.008</b>	<b>4.008</b>
$VB2$	2.2214	2.0391	1.9111	2.3419	2.2175	2.0058	<b>2.405</b>	<b>2.405</b>
$D1$	0.5570	0.5798	0.5802	0.5524	0.6079	0.6005	0.6026	0.6116
$D2$	0.2546	0.2452	0.2334	0.2610	0.2582	0.2417	0.2685	0.2683
$B1$	0.8030	0.8202	0.8198	0.8076	0.8621	0.8495	0.8574	0.8684
$B2$	0.5484	0.5751	0.5865	0.5467	0.6039	0.6079	0.5888	0.6001
$x_A$	0.9594	<b>0.95</b>	<b>0.95</b>	0.9667	<b>0.95</b>	<b>0.95</b>	0.9517	<b>0.95</b>
$x_B$	<b>0.95</b>	<b>0.95</b>	<b>0.95</b>	<b>0.95</b>	<b>0.95</b>	<b>0.95</b>	<b>0.95</b>	<b>0.95</b>
$x_c$	0.9862	0.9685	<b>0.95</b>	0.9896	0.9697	<b>0.95</b>	0.9867	0.9824
$J$	-0.0715	0.2863	0.6952	-0.1340	0.3643	0.96108	-0.2044	-0.1401

## 4.2 Self – optimizing variables

The scaled gains of the stage temperatures in each region of the three different case studies were found according to the Minimum Singular Value Rule. The temperatures with the largest scaled gains were chosen as self – optimizing variables. The Exact Local Method was used to find combinations of stage temperatures as self – optimizing variables.

The pairing of active constraints and self – optimizing variables with the degrees of freedom, along with the their optimal values for the different case studies, are shown in Appendix B.

### 4.2.1 Minimum Singular Value Rule

#### 4.2.2 Case Study 1a

As seen in Figure 4.1, only region I has unconstrained degrees of freedom after the active constraints are controlled. The reflux,  $L$ , was assumed to control the active constraint, while the boilup,  $V$ , was used for self – optimizing control. A presentation of the scaled gains are given in Figure 4.4. The scaled gain is largest at stage number 11.

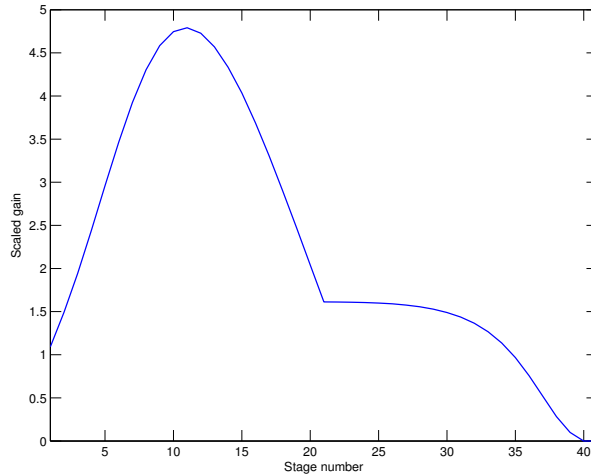


Figure 4.4: Scaled gains for case study 1a.

### 4.2.3 Case Study 1b

The three regions I, IV and V in Figure 4.2, have unconstrained degrees of freedom left after controlling the active constraints. The scaled gains for each region are shown in Figure 4.5

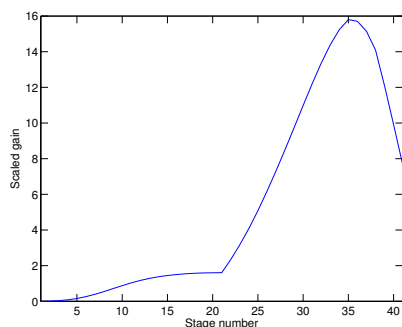
In region I, the boilup,  $V$ , was assumed to be controlling the active constraint, while the reflux,  $L$ , was used for self – optimizing control. The boilup,  $V$ , was at its active constraint value in region IV, which left the reflux,  $L$ , for self – optimizing control. The last region, V, has no active constraints. Both the boilup,  $V$ , and the reflux  $L$  are free for self – optimizing control.

The largest scaled gain in region I is stage 35. In region IV stage 14 has the largest scaled gain, while the largest scaled gain for region V is at stage 32 for both perturbations in reflux and boilup.

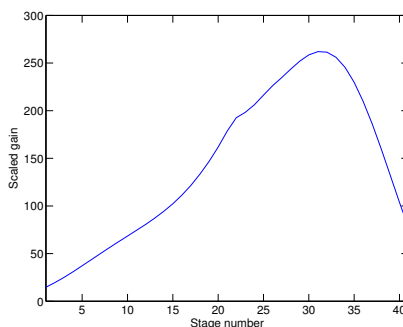
### 4.2.4 Case Study 2

There are 6 regions, I, II, III, IV, V and VII, with unconstrained degrees of freedom in case study 2.

In region I the reflux of column 2,  $L2$ , was assumed to be controlling the active constraint, while the reflux of column 1,  $L1$  and the boilups,  $V1$  and  $V2$ , were used for self – optimizing control. The scaled gains can be seen in Figure 4.6. The largest scaled gain for a perturbation in  $L1$  is at stage 32 in column 1. Stage 13



(a) Region I.



(b) Region IV.

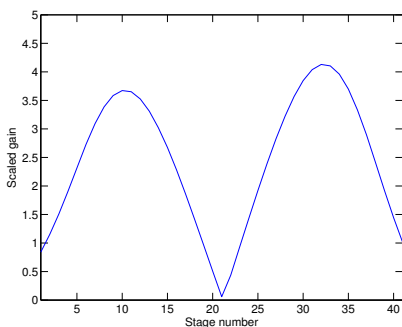
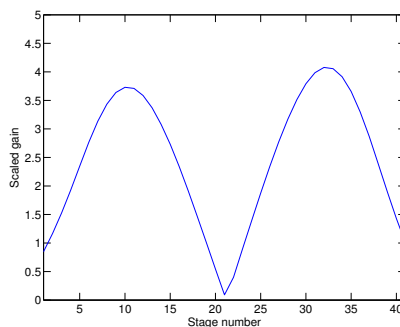
(c) Region V with perturbation in  $L$ .(d) Region V with perturbation in  $V$ .

Figure 4.5: Scaled gains for regions (a) I, (b) IV and (c)(d) V.

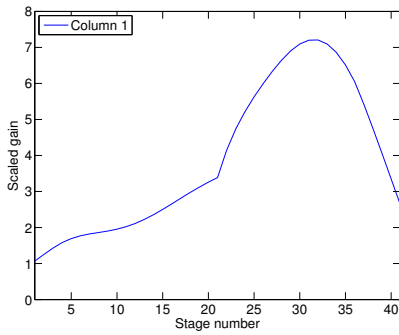
in column 1 has the largest scaled gain for a perturbation in  $V1$ , and stage 13 in column 2 has the largest gain for a perturbation in  $V2$ .

In region II both refluxes,  $L1$  and  $L2$ , are assumed to control the active constraints. The remaining degrees of freedom are the boilups,  $V1$  and  $V2$ . They are used for self – optimizing control. The scaled gains for this region are shown in Figure 4.7. The largest scaled gain for a perturbation in  $V1$  is at stage 12 in column 1, and for  $V2$  at stage 9 in column 2.

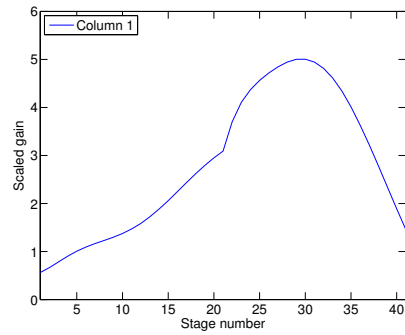
In region III, the refluxes,  $L1$  and  $L2$ , and the boilup,  $V2$ , are assumed to control the active constraints. The reflux,  $V1$ , was used for self – optimizing control. The resulting scaled gains are shown in Figure 4.8. The largest scaled gain for a perturbation in  $V1$  is at stage 13 in column 1.

The reflux of column 2,  $L2$ , and boilup of column 1,  $V1$ , control the active constraints in region IV. This leaves the reflux of column 1,  $L1$ , and boilup of column

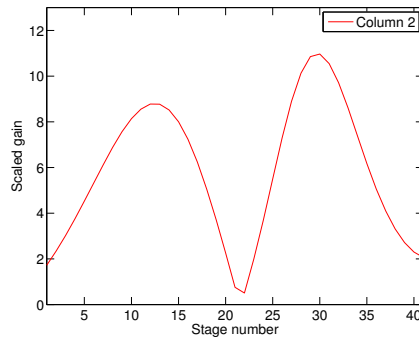




(a) Perturbation in L1.

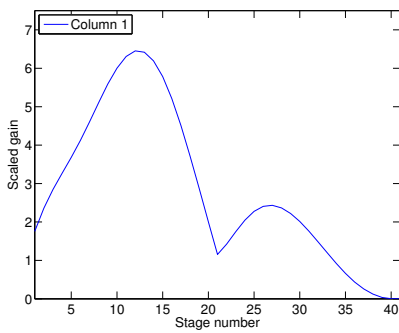


(b) Perturbation in V1.

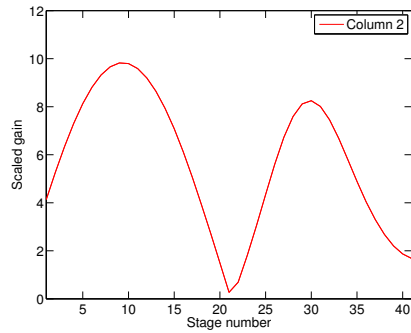


(c) Perturbation in V2.

Figure 4.6: Scaled gains for region I



(a) Perturbation in V1.



(b) Perturbation in V2.

Figure 4.7: Scaled gains for region II.

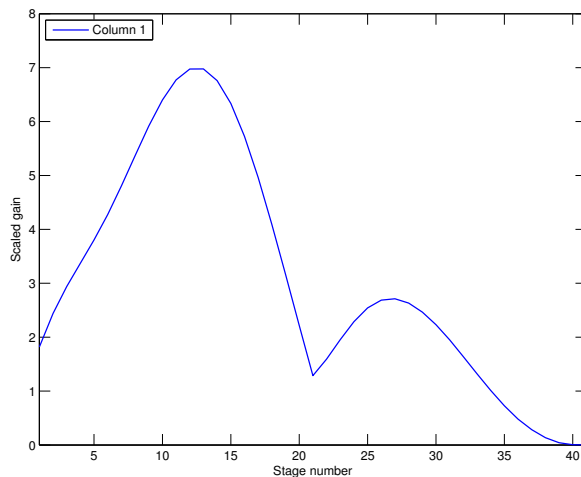
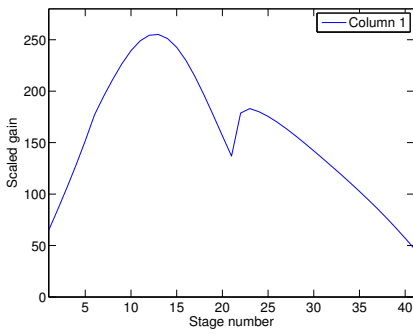


Figure 4.8: Scaled gain for region III.

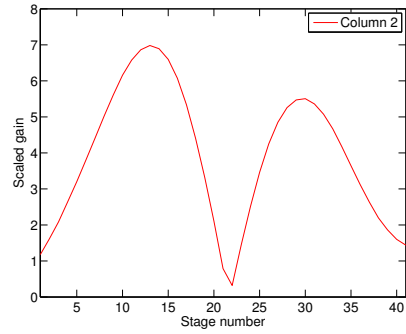
2,  $V2$ , for self – optimizing control. The resulting scaled gains are shown in Figure 4.9. The largest scaled gain for a perturbation in  $L1$  is at stage 14 in column 1, and the largest scaled gain for a perturbation in  $V2$  is at stage 13 in column 2.

Both the refluxes,  $L1$  and  $L2$ , are assumed to control the active constraints in region V. The boilups of column 1 and 2,  $V1$  and  $V2$ , were used for self – optimizing control. The resulting scaled gains are shown in Figure 4.10. The largest scaled gain are at stage 13 of column 1.

In region VII the boilups,  $V1$  and  $V2$ , and the reflux of column 2,  $L2$ , control the active constraints. The reflux of column 1,  $L1$ , was used for self – optimizing control. The resulting scaled gains are shown in Figure 4.11. The largest scaled gain for  $L1$  is at stage 13 in column 1.



(a) Perturbation L1



(b) Perturbation V2

Figure 4.9: Scaled gains for region IV.

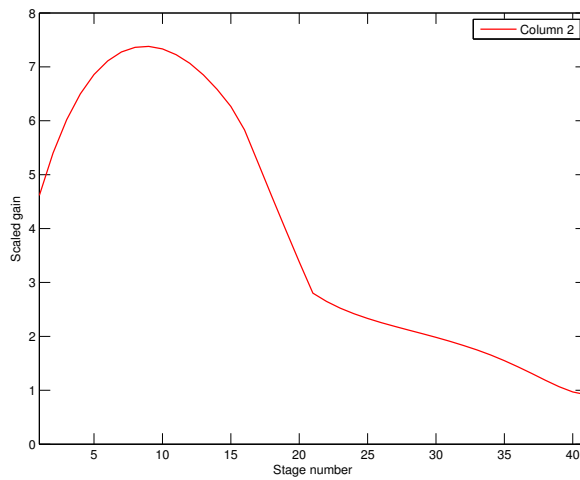


Figure 4.10: Scaled gain for region V.

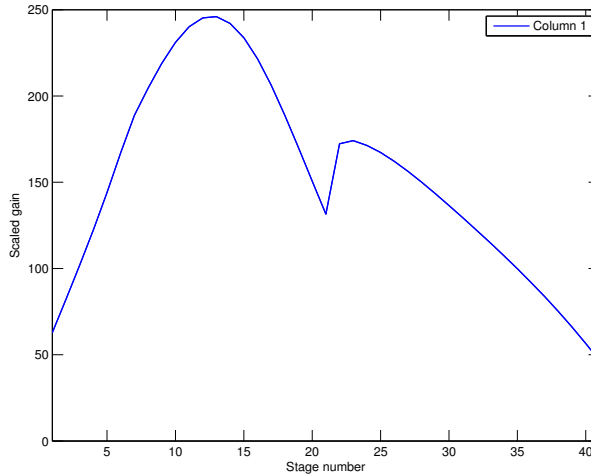


Figure 4.11: Scaled gains for region VII.

#### 4.2.5 Exact Local Method

The Exact Local Method was used to find optimal combinations of temperatures as self – optimizing variables. Both a combination of all temperatures and temperatures at every 5th stage were considered. In this section only the combinations of every 5th temperature of case studies 1a and 1b are shown in Table 4.4. The results in its entirety are presented in Appendix A.

Table 4.4: Combination of temperatures at every 5th stage as candidate variables in each region for the case studies 1a and 1b.

Temperature	Case 1a		Case 1b		
	Region I	Region I	Region IV	Region $V - u = L$	Region $V - u = V$
$T_5$	1	-0.0097	0.3626	1	1
$T_{10}$	2.3889	-0.0875	1	2.7813	2.7635
$T_{15}$	2.6278	-0.2825	0.936	3.8269	3.7548
$T_{20}$	-0.3405	-0.4207	-0.9376	1.0215	0.9085
$T_{25}$	-0.9962	0.0649	0.2764	-2.9444	-2.8345
$T_{30}$	-0.7345	0.8745	0.9513	-4.0572	-3.83
$T_{35}$	-0.2386	1	0.5228	-2.1086	-1.9774
$T_{40}$	0	0.3958	0.1428	-0.5702	-0.5337

## 4.3 Simulations

A selection of the control structures for the different regions for each case study were tested on the dynamic nonlinear models in Matlab/Simulink. The tested self – optimizing variables were a single stage temperature, a combination of all stage temperatures and a combination of every 5th stage temperature.

For case studies 1a and b, disturbances occurred at:

- $t = 300$  min, increase in feed flow rate by 20% .
- $t = 700$  min, increase in feed composition by 10%.
- $t = 1100$  min, decrease in liquid composition by 10%.

For case study 2, disturbances occurred at:

- $t = 200$  min, increase in feed flow rate by 0.01 kmol/min.
- $t = 400$  min, decrease in liquid composition by 10%.

### 4.3.1 Case Study 1a

The testing of the candidate variables for case study 1a is shown in Figure 4.12.

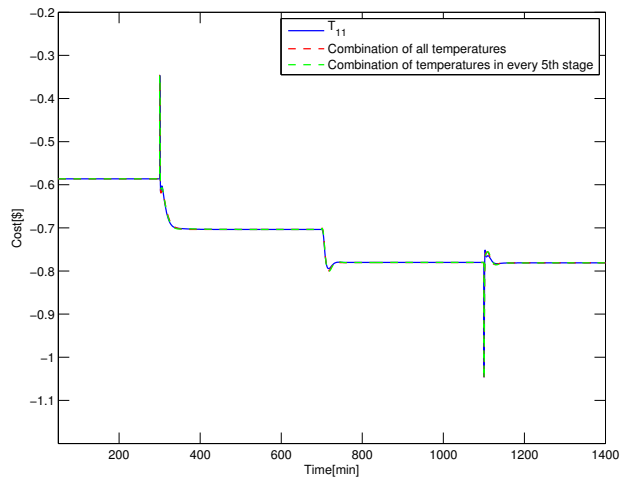


Figure 4.12: Simulation of region I.

The cost function follows the same trajectory for all the self – optimizing variables when controlling them to a constant optimal value.

### 4.3.2 Case Study 1b

The simulation of region I is shown below in Figure 4.13

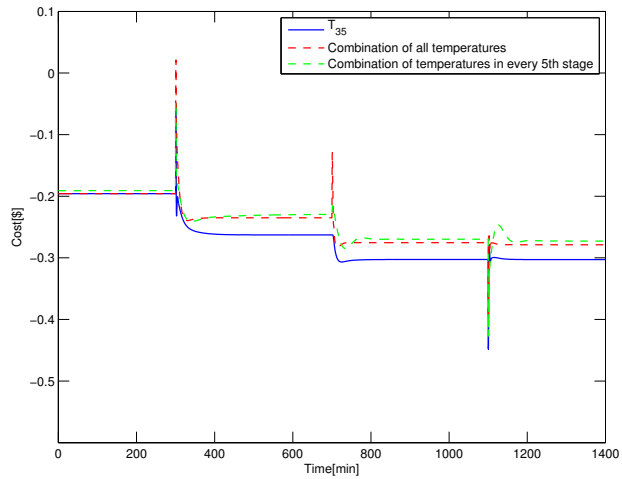


Figure 4.13: Simulation of region I.

As seen from the figure, controlling the combinations of temperatures yields a higher cost than controlling only the temperature at stage 35.

The testing of the self – optimizing variables for Region IV are shown in Figure 4.14.

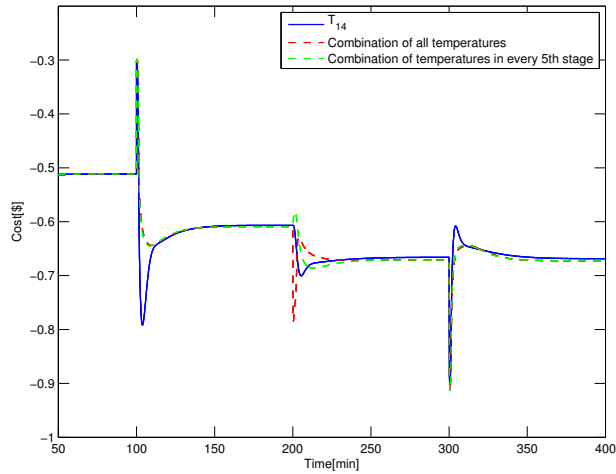


Figure 4.14: Simulation of region IV.

Controlling a combination of temperatures at every 5th stage deals better with incoming disturbances than the other two self – optimizing variables.

### 4.3.3 Case Study 2

The testing of the self – optimizing variables for regions III and VII are shown in Figure 4.15. The cost functions in both simulations seem to follow the same trajectory for all the self – optimizing variables.

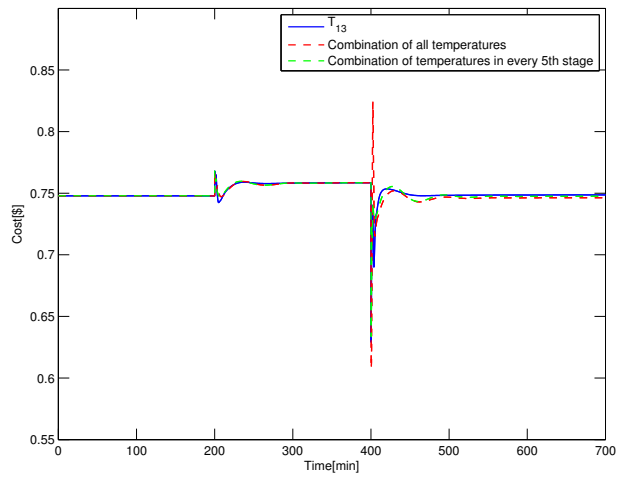


Figure 4.15: Simulation of region III.

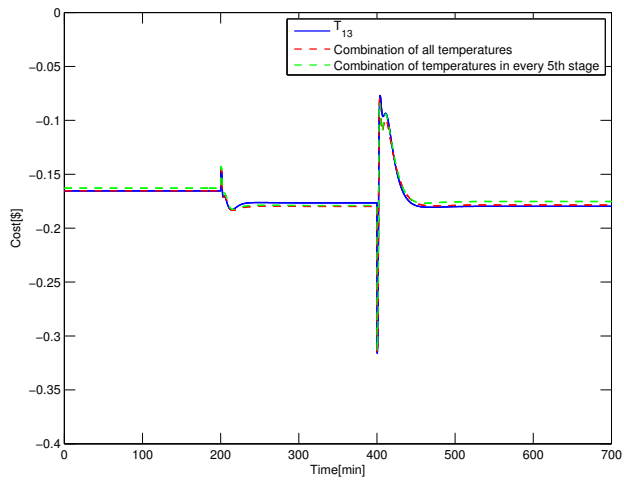


Figure 4.16: Simulation of region VII.



# Chapter 5

## Discussion

In this chapter the results and procedures will be explained and discussed.

### 5.1 Maps of the Active Constraint Regions

The maps of the active constraint regions were found by optimizing the models with a sequential increase in the disturbances. The model was solved by setting the state derivatives equal to zero.

In all regions of case study 1a,  $x_D = x_{D,min}$ . This follows the *Product giveaway rule* (Skogestad 2007). A chemical company will not benefit from selling a product with purity above the required specification when the product price is fixed and over purifying costs extra. Exactly the same is valid for case study 2 and the valuable product B,  $x_B = x_{B,min}$ .

There are three active constraint regions in case study 1, mapped in Figure 4.1. By increasing the feed flow rate, the internal flows,  $L$  and  $V$ , will increase up to a point where  $V = V_{max}$ . A further increase will violate the purity constraints, thus making the process infeasible. When the energy price is low it is beneficial to over purify the bottom product due to its low value opposed to the distillate. Over purifying the bottom moves more valuable product to the top. Higher energy prices makes this costly and the constraint for the purity of the bottom becomes active. Also, with higher prices less energy is used to send component A to the top and therefore more feed is needed before the constraint for boilup becomes active. This is seen from the red line between the regions I and III.

There are five active constraint regions in case study 1b. These were mapped in Figure 4.2. As the distillate price is now proportional to purity, the energy price needs to be substantially high before the constraint of distillate purity becomes active. Low energy prices makes it optimal to over purify both the distillate and the bottom products. Since the the distillate is the most valuable product the bot-

tom product reaches its active constraint value before the distillate. An interesting property for this case study is that the constraint for bottom product purity becomes active when increasing the feed flow rate from region IV to region III. With the boilup already being at its maximum, a further increase in the feed flow rate will activate the bottom product constraint because of the low value of component B.

Case study 2 gives rise to 8 different active constraint regions. The purity constraints follow the trends as seen in the two other maps – increasing the energy price the over purification of distillate and bottom products is too expensive and the purity constraints become active. With low energy prices, more of components A and B are pushed to the top of column 1 and 2, respectively, and the boilups reaches their active constraint values. The constraint line separating regions II and V has a negative slope. This indicates that the optimal values for the boilup of column 1 will increase with increasing energy prices. This do not coincide with the trends seen in the other two cases. However,  $V_2$  is decreasing and also the sum of  $V_1 + V_2$  is decreasing as a counter measure. Another interesting feature is the curved constraint line for  $x_C$  separating the regions V and VI. All other purity constraint lines are horizontal. An increase in the feed while  $V_1 = V_{1,max}$ , will make more of component A flow to column 2, and therefore increasing the amount component C in the bottom of column 2, making the constraint active.

### 5.1.1 Comparison With Previous Work

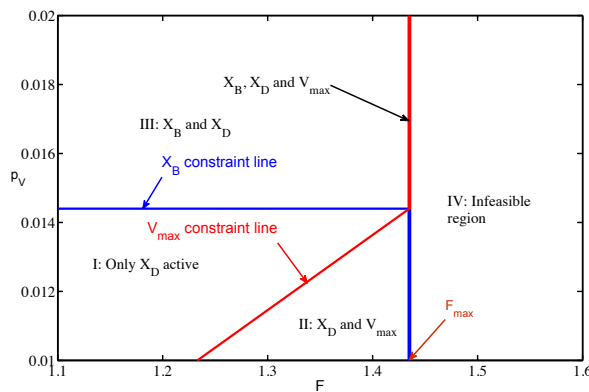


Figure 5.1: Active constraint region for a single distillation column with constant prices (Jacobsen 2011).

Comparison of the active constraint map for case study 1a constructed in this work

with previous results seen in Figure 5.1 (Jacobsen 2011), shows some differences. The main difference is the line separating the active constraint regions  $x_D - x_D, x_B$ . This constraint line is at a larger energy price in this work than in Jacobsen's. The reason for this is shown in Jacobsen's Matlab code, where stage 20 is used for the feed inlet. This pushes the active constraint line downwards.

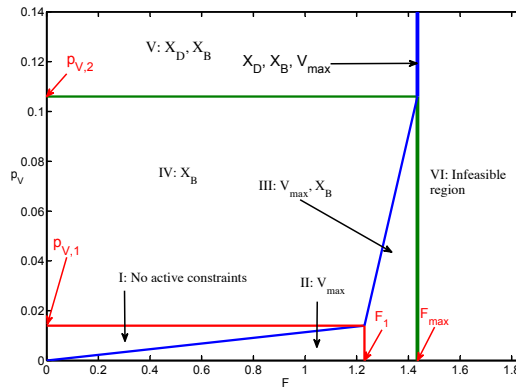


Figure 5.2: Active constraint region for a single distillation column with purity dependent prices (Jacobsen 2011).

The active constraint regions for case study 1b in this work and the corresponding by Jacoben (2011), Figure 5.2, are close to equal. The constraint lines separating regions I and II (actually region IV and V in this work) is curved. This is because Jacobsen, when drawing the constraint lines, only uses two points, and therefore lacks the curved trends the lines have.

The map for case study 2 in this work and in Jacobsen (2011) seems to be identical, as seen from Figure 5.3.

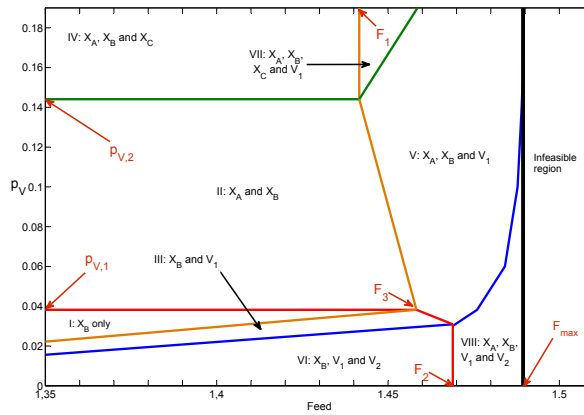


Figure 5.3: Active constraint region for two distillation columns in sequence with constant prices (Jacobsen 2011).

## 5.2 Minimum Singular Value Rule

The stage temperatures, with the largest scaled gain for each case study, was chosen as self – optimizing variables when using the Minimum Singular Value Rule. This rule generally overestimates the worst – case loss because of the assumption that any output deviation satisfying that the combined errors of the 2 – norm is less than 1, is allowed (Halvorsen et al. 2003). This implies that more than the temperature with the best scaled gain should be further investigated as self – optimizing variables.

The stage temperatures found in each region of the case studies are concentrated between the ends of the column and the feed inlet at stage 21. For most of the regions, the temperature controlled should be put to stages 9 –14 when boilup is the unconstrained degree of freedom, and stage 30 – 35 when reflux is the unconstrained degree of freedom. The results found coincide with the temperature profiles shown in Appendix C.

For two distillation columns in sequence, the concentration of bottom product of column 1 should rather be used as a controlled variable than using temperatures. Variations in the concentration of the flow that enters column 2 may cause troubles for column 1, when only controlling the temperatures.

## 5.3 Simulations

Three simulations were done to compare the different control structures in the case studies 1a and 1b. Two simulations were done for case study 2. Of the five simulations, case study 1b, region I, points out. Controlling the temperature in stage 35 opposed to controlling combinations of temperatures gives different costs after the feed flow rate is increased. The process operates with better profit after disturbances are introduced by using the temperature at stage 35 as a self – optimizing variable.

The simulations done in this work is only to demonstrate the applicability of the self – optimizing control structures found. A much more detailed analysis of the different alternatives is needed before choosing the optimal control structures.

## 5.4 Ipopt/sIpopt

The software package Ipopt/sIpopt was used for optimization of the case studies, and for calculating the optimal sensitivities of the measurements with respect to disturbances. The optimal sensitivities are used in both the Minimum Singular Value Rule and the Exact Local method, thus making Ipopt/sIpopt a useful tool for self – optimizing control studies.



# Chapter 6

## Conclusion

The active constraint regions for each of the three case studies have been identified and mapped with respect to the disturbances; energy price and feed flow rate. Stage temperatures and combinations of stage temperatures have been proposed as self – optimizing variables for the unconstrained degrees of freedom of each region. A selection of the proposed control structures for the different regions of each case study have been implemented and compared on the dynamic nonlinear models using Simulink.

It has been shown that the first case study, a single distillation column with constant product prices, has 3 active constraint regions. The next case study, a single distillation column with purity dependent prices, has 5 active constraint regions, while the last case study, two columns in sequence with constant prices, has 8 active constraint regions.

The optimal sensitivities of the measurements with respect to disturbances, was easily calculated by using the software package Ipopt/sIpopt.





## Chapter 7

# Further Work

The continuation of this work should be to thoroughly test the different self – optimizing control structures proposed.

One should also test control other variables than only stage temperatures as candidates for self – optimizing control. I.e. a combination of reflux and temperatures which has proved a good alternative (Hori & Skogestad 2007). Other combinations like flows and flow ratios may also be considered.

In case study 2, an interesting controlled variable to check is the amount of component A that is carried from column 1 to column 2. Keeping it constant may remove the problem arising in column 2 when large variations of concentration flow through it from column 1 (Jacobsen 2011).



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# Appendix A

## Combinations of temperatures as self – optimizing variables

The combinations of temperatures as self – optimizing variables ( $H$  – matrix) are listed in the tables below.

Table A.1: Combination of temperatures at every 5th stage as self – optimizing variables for the case studies 1a and 1b.

Temperature	Case 1a		Case 1b		
	Region I	Region I	Region IV	Region $V - u = L$	Region $V - u = V$
$T_5$	1	-0.0097	0.3626	1	1
$T_{10}$	2.3889	-0.0875	1	2.7813	2.7635
$T_{15}$	2.6278	-0.2825	0.936	3.8269	3.7548
$T_{20}$	-0.3405	-0.4207	-0.9376	1.0215	0.9085
$T_{25}$	-0.9962	0.0649	0.2764	-2.9444	-2.8345
$T_{30}$	-0.7345	0.8745	0.9513	-4.0572	-3.83
$T_{35}$	-0.2386	1	0.5228	-2.1086	-1.9774
$T_{40}$	0	0.3958	0.1428	-0.5702	-0.5337

Table A.2: Combination of all temperatures as self – optimizing variables for the case studies 1a and 1b.

Temperature	Case 1a		Case 1b		
	Region I	Region I	Region IV	Region $V - u = L$	Region $V - u = V$
$T_1$	1	0	0.1139	-0.0557	0.0712
$T_2$	1.402	-0.0005	0.1612	-0.0808	0.1047
$T_3$	1.8748	-0.002	0.2205	-0.1102	0.1424
$T_4$	2.4411	-0.0049	0.2937	-0.1478	0.1883
$T_5$	3.089	-0.0095	0.383	-0.1904	0.2453
$T_6$	3.8306	-0.0166	0.4895	-0.2463	0.3131
$T_7$	4.6659	-0.027	0.6133	-0.3106	0.3925
$T_8$	5.5571	-0.0415	0.7517	-0.3847	0.4846
$T_9$	6.4809	-0.0608	0.8979	-0.4687	0.5888
$T_{10}$	7.3626	-0.0856	1.0397	-0.5578	0.6949
$T_{11}$	8.1347	-0.1161	1.1581	-0.6506	0.8034
$T_{12}$	8.6912	-0.1519	1.2281	-0.7336	0.8972
$T_{13}$	8.921	-0.1919	1.2216	-0.8007	0.9683
$T_{14}$	8.7339	-0.2342	1.1135	-0.8378	1
$T_{15}$	8.0591	-0.2765	0.8905	-0.8395	0.9863
$T_{16}$	6.859	-0.316	0.5579	-0.7984	0.9188
$T_{17}$	5.2087	-0.3504	0.1422	-0.7142	0.7989
$T_{18}$	3.188	-0.3782	-0.3144	-0.5924	0.6343
$T_{19}$	0.9441	-0.3986	-0.7656	-0.4485	0.4447
$T_{20}$	-1.3631	-0.4118	-1.1722	-0.2944	0.2429
$T_{21}$	-3.5931	-0.4187	-1.5097	-0.141	0.0466
$T_{22}$	-3.5789	-0.3273	-1.0746	0.0702	-0.1612
$T_{23}$	-3.5556	-0.2194	-0.6278	0.2881	-0.3782
$T_{24}$	-3.5082	-0.0949	-0.1964	0.499	-0.5843
$T_{25}$	-3.4402	0.0454	0.1923	0.6871	-0.7641
$T_{26}$	-3.3358	0.1987	0.5152	0.8385	-0.9073
$T_{27}$	-3.2041	0.3598	0.7574	0.9439	-1.0025
$T_{28}$	-3.0274	0.5212	0.9144	0.9973	-1.0449
$T_{29}$	-2.7986	0.6737	0.9912	1	-1.0354
$T_{30}$	-2.5345	0.8066	1	0.9602	-0.9871
$T_{31}$	-2.2147	0.91	0.9569	0.8895	-0.9072
$T_{32}$	-1.8697	0.9759	0.8785	0.7975	-0.8095
$T_{33}$	-1.5115	1	0.7796	0.6935	-0.6998
$T_{34}$	-1.1525	0.9822	0.6721	0.5889	-0.5931
$T_{35}$	-0.82	0.9265	0.5646	0.4907	-0.49
$T_{36}$	-0.54	0.8403	0.4627	0.3973	-0.3947
$T_{37}$	-0.3108	0.7325	0.3699	0.3165	-0.3133
$T_{38}$	-0.1499	0.6125	0.2877	0.2451	-0.2418
$T_{39}$	-0.0411	0.4884	0.2163	0.1821	-0.1809
$T_{40}$	0	0.3668	0.1554	0.1308	-0.1293
$T_{41}$	0	0.2524	0.1041	0.0877	-0.0875

Table A.3: Combination of every 5th temperature as self – optimizing variables the for regions I and II, case study 2.

Temp	Region I			Region II	
	$u = L1$	$u = V1$	$u = V2$	$u = V1$	$u = V2$
$T_5$	1	1	1	1	1
$T_{10}$	2.1653	2.1568	1.8566	1.8025	1.3151
$T_{15}$	1.9204	1.9167	1.7784	1.7157	0.8019
$T_{20}$	-0.7542	-0.7341	0.3197	-0.1634	0.0291
$T_{25}$	-1.6187	-1.5548	-3.6481	0.2227	-0.809
$T_{30}$	-2.1064	-2.0222	-6.5365	0.3615	-1.2955
$T_{35}$	-2.0223	-1.9523	-3.5676	0.1116	-0.694
$T_{40}$	-1.0273	-0.9931	-1.3053	-0.0005	-0.2543

Table A.4: Combination of all temperatures as self – optimizing variables for the regions I and II, case study 2.

Temp	I			Region II	
	$u = L1$	$u = V1$	$u = V2$	$u = V1$	$u = V2$
$T_1$	1	1	1	1	1
$T_2$	1.3294	1.3376	1.3219	1.2282	1.3342
$T_3$	1.5653	1.5783	1.5406	1.4198	1.6715
$T_4$	1.763	1.7726	1.713	1.5919	1.9991
$T_5$	1.9724	1.9748	1.8914	1.7598	2.301
$T_6$	2.2251	2.2376	2.1185	1.9329	2.5601
$T_7$	2.5464	2.5486	2.4002	2.1108	2.7587
$T_8$	2.9025	2.907	2.7122	2.2865	2.88
$T_9$	3.259	3.266	3.0314	2.4424	2.9147
$T_{10}$	3.5658	3.5721	3.3043	2.5581	2.855
$T_{11}$	3.7804	3.7852	3.4856	2.6142	2.7033
$T_{12}$	3.8446	3.8508	3.5279	2.5916	2.4648
$T_{13}$	3.7052	3.7112	3.3995	2.476	2.1555
$T_{14}$	3.3748	3.3777	3.0754	2.2613	1.7903
$T_{15}$	2.8346	2.8395	2.5646	1.9465	1.3903
$T_{16}$	2.1033	2.0989	1.8785	1.5422	0.971
$T_{17}$	1.2183	1.2203	1.0582	1.0627	0.5496
$T_{18}$	0.2289	0.2272	0.141	0.5306	0.1376
$T_{19}$	-0.804	-0.8084	-0.8185	-0.0334	-0.2531
$T_{20}$	-1.8499	-1.8578	-1.7727	-0.6069	-0.6208
$T_{21}$	-2.8486	-2.8572	-2.6986	-1.1726	-0.9625
$T_{22}$	-2.5416	-2.5409	-2.2509	-0.9075	-1.6052
$T_{23}$	-2.1314	-2.1253	-1.7436	-0.8127	-2.3437
$T_{24}$	-1.7464	-1.7371	-1.2831	-0.8813	-3.1457
$T_{25}$	-1.4614	-1.4448	-0.9238	-1.0694	-3.9635
$T_{26}$	-1.2759	-1.2564	-0.6837	-1.3123	-4.7246
$T_{27}$	-1.1883	-1.1676	-0.5474	-1.5381	-5.3483
$T_{28}$	-1.1681	-1.1498	-0.4901	-1.6806	-5.7606
$T_{29}$	-1.197	-1.1722	-0.4861	-1.6967	-5.9108
$T_{30}$	-1.2403	-1.2116	-0.5094	-1.5684	-5.7923
$T_{31}$	-1.2816	-1.2544	-0.5456	-1.3132	-5.4372
$T_{32}$	-1.3151	-1.2883	-0.5827	-0.9728	-4.91
$T_{33}$	-1.3152	-1.2895	-0.6075	-0.5986	-4.2835
$T_{34}$	-1.2858	-1.2684	-0.6201	-0.2416	-3.6297
$T_{35}$	-1.2345	-1.2156	-0.6097	0.06	-3.0039
$T_{36}$	-1.1564	-1.132	-0.5866	0.2836	-2.4403
$T_{37}$	-1.0439	-1.0308	-0.5473	0.4186	-1.9638
$T_{38}$	-0.9194	-0.9079	-0.4953	0.4657	-1.577
$T_{39}$	-0.7863	-0.7717	-0.4257	0.431	-1.2841
$T_{40}$	-0.6422	-0.633	-0.3493	0.3227	-1.0824
$T_{41}$	-0.4907	-0.4859	-0.2676	0.1515	-0.9707



Table A.5: Combination of every 5th temperature as self – optimizing variables for the regions III, IV, V and VII, case study 2.

Temp	Region III	Region IV		Region V	Region VII
	$u = V1$	$u = L1$	$u = V2$	$u = V2$	$u = L1$
$T_5$	1	1	1	1	1
$T_{10}$	1.8437	1.8885	2.0303	1.431	1.8675
$T_{15}$	1.8224	1.8781	2.2291	0.9918	2.0853
$T_{20}$	-0.1336	-0.2186	0.7461	0.1803	1.2389
$T_{25}$	0.2778	-0.2828	-1.0365	-0.4353	1.215
$T_{30}$	0.4077	-0.2485	-2.1143	-0.6829	0.9381
$T_{35}$	0.1252	-0.3205	-1.1058	-0.3383	0.4987
$T_{40}$	-0.0011	-0.1745	-0.4249	-0.123	0.1782

Table A.6: Combination of all temperatures as a self – optimizing variables for the regions III, IV, V and VII, case study 2.

Temp	Region III	Region IV		Region V	Region VII
	$u = V1$	$u = L1$	$u = V2$	$u = V2$	$u = L1$
$T_1$	1	1	1	1	1
$T_2$	1.2728	1.2493	1.1626	1.246	1.3896
$T_3$	1.4311	1.3732	1.2755	1.4896	1.7624
$T_4$	1.5364	1.4342	1.3877	1.7218	2.1329
$T_5$	1.6464	1.4997	1.4702	1.9214	2.52
$T_6$	1.8022	1.6168	1.5627	2.0605	2.9352
$T_7$	2.0203	1.8036	1.6546	2.1106	3.3775
$T_8$	2.2863	2.0519	1.7561	2.0491	3.8313
$T_9$	2.5707	2.334	1.8538	1.8629	4.2695
$T_{10}$	2.8322	2.6104	1.9469	1.554	4.6574
$T_{11}$	3.0258	2.8357	1.9892	1.1409	4.9572
$T_{12}$	3.1027	2.9642	1.9939	0.6554	5.1341
$T_{13}$	3.0301	2.9551	1.9378	0.138	5.1612
$T_{14}$	2.779	2.7785	1.7946	-0.368	5.0247
$T_{15}$	2.3464	2.4194	1.5686	-0.823	4.7251
$T_{16}$	1.7417	1.8805	1.2466	-1.1991	4.2786
$T_{17}$	0.9922	1.1815	0.8334	-1.4819	3.7141
$T_{18}$	0.1356	0.3567	0.3415	-1.6681	3.0666
$T_{19}$	-0.7816	-0.5513	-0.2076	-1.7676	2.3747
$T_{20}$	-1.7144	-1.4972	-0.7928	-1.7966	1.6731
$T_{21}$	-2.6261	-2.439	-1.4155	-1.7735	0.9915
$T_{22}$	-2.0481	-2.1213	-1.077	-1.2108	1.2106
$T_{23}$	-1.4207	-1.6802	-1.037	-0.6266	1.4137
$T_{24}$	-0.8525	-1.2371	-1.2402	-0.0449	1.558
$T_{25}$	-0.395	-0.8624	-1.5995	0.5009	1.6255
$T_{26}$	-0.0636	-0.5799	-1.999	0.9705	1.6169
$T_{27}$	0.1526	-0.3837	-2.3159	1.3261	1.5438
$T_{28}$	0.2784	-0.255	-2.466	1.5451	1.4217
$T_{29}$	0.3345	-0.1737	-2.3864	1.6264	1.266
$T_{30}$	0.3435	-0.123	-2.0887	1.5917	1.0918
$T_{31}$	0.3213	-0.0904	-1.5955	1.4773	0.9111
$T_{32}$	0.2776	-0.0686	-1.0083	1.3203	0.7342
$T_{33}$	0.2266	-0.0532	-0.4002	1.1539	0.5693
$T_{34}$	0.1747	-0.0416	0.161	0.9982	0.422
$T_{35}$	0.1252	-0.0325	0.6004	0.8628	0.2963
$T_{36}$	0.0812	-0.0254	0.8937	0.7493	0.1938
$T_{37}$	0.0477	-0.019	1.0429	0.6539	0.1153
$T_{38}$	0.022	-0.0126	1.0626	0.5733	0.0591
$T_{39}$	0.0066	-0.0048	0.9438	0.5031	0.0234
$T_{40}$	-0.002	0.005	0.7356	0.4427	0.0057
$T_{41}$	-0.001	0.0178	0.4384	0.3948	0.0032

# Appendix B

## Pairing

The pairing of the active constraints and self – optimizing variables with the degrees of freedom are shown in the tables below. The optimal values of the variables are also listed.

### B.1 Case study 1a

Table B.1: Pairing of active constraints/self – optimizing variables with degrees of freedom, case study 1a.

Active constraints/ self – optimizing variables	DOF	fixed values
$x_D$	$L$	0.95
$T_{11}$	$V$	380.197 [°C]
Comb all	$V$	2.093e+04 [°C]
Comb 5th	$V$	1.433e+03 [°C]

## B.2 Case study 1b

Table B.2: Region I, case study 1b.

Active constraints/ self – optimizing variables	DOF	fixed values
$x_B$	$V$	0.99
$T_{35}$	$L$	358.582 [°C]
Comb all	$L$	2.311e+03 [°C]
Comb 5th	$L$	542.155 [°C]

Table B.3: Region IV, case study 1b.

Active constraints/ self – optimizing variables	DOF	fixed values
$V_{max}$	$V$	4.008 [kmol/min]
$T_{35}$	$L$	353.466 [°C]
Comb all	$L$	4.798e+03 [°C]
Comb 5th	$L$	51.579e+03 [°C]

Table B.4: Region V, case study 1b.

Active constraints/ self – optimizing variables	DOF	fixed values
$T_{32}$	$L$	356.868 [°C]
Comb all	$L$	443.092 [°C]
Comb 5th	$L$	-222.039 [°C]
$T_{32}$	$V$	356.868 [°C]
Comb all	$V$	-995.682 [°C]
Comb 5th	$V$	-116.635 [°C]

## B.3 Case study 2

Table B.5: Region I, case study 2.

Active constraints/ self – optimizing variables	DOF	fixed values
$x_B$	$L2$	0.95
<b>Column 1</b>		
$T_{32}$	$L1$	359.619 [°C]
Comb all	$L1$	5.466e+03 [°C]
Comb 5th	$L1$	-760.788 [°C]
$T_{30}$	$V1$	361.219 [°C]
Comb all	$V1$	5.614e+03 [°C]
Comb 5th	$V1$	-666.933 [°C]
<b>Column 2</b>		
$T_{30}$	$V2$	391.589 [°C]
Comb all	$V2$	7.948e+03 [°C]
Comb 5th	$V2$	-3.873e+03 [°C]

Table B.6: Region II, case study 2.

Active constraints/ self – optimizing variables	DOF	fixed values
$x_A$	$L1$	0.95
$x_B$	$L2$	0.95
<b>Column 1</b>		
$T_{12}$	$V1$	385.826 [°C]
Comb all	$V1$	1.067e+04 [°C]
Comb 5th	$V1$	1.941e+03 [°C]
<b>Column 2</b>		
$T_9$	$V2$	406.974 [°C]
Comb all	$V2$	-1.3821e+04 [°C]
Comb 5th	$V2$	84.6756 [°C]

Table B.7: Region III, case study 2.

Active constraints/ self – optimizing variables	DOF	fixed values
$x_A$	$L1$	0.95
$x_B$	$L2$	0.95
$x_C$	$V2$	0.95
<b>Column 1</b>		
$T_{13}$	$V1$	384.901 [°C]
Comb all	$V1$	1.097e+04 [°C]
Comb 5th	$V1$	2.051e+03 [°C]

Table B.8: Region IV, case study 2.

Active constraints/ self – optimizing variables	DOF	fixed values
$V1_{max}$	V1	4.008
$x_B$	L2	0.95
<b>Column 1</b>		
$T_{14}$	L1	382.853 [°C]
Comb all	L1	8.770e+03 [°C]
Comb 5th	L1	1.390e+03 [°C]
<b>Column 2</b>		
$T_{13}$	V2	407.379 [°C]
Comb all	V2	4.645e+03 [°C]
Comb 5th	V2	617.527 [°C]

Table B.9: Region V, case study 2.

Active constraints/ self – optimizing variables	DOF	fixed values
$V1_{max}$	V1	4.008
$x_A$	L1	0.95
$x_B$	L2	0.95
<b>Column 1</b>		
$T_9$	V2	406.984 [°C]
Comb all	V2	9.101e+03 [°C]
Comb 5th	V2	846.596 [°C]

Table B.10: Region VII, case study 2.

Active constraints/ self – optimizing variables	DOF	fixed values
$V1_{max}$	$V1$	4.008
$V2_{max}$	$V2$	0.95
$x_B$	$L2$	0.95
<b>Column 1</b>		
$T_{13}$	$L1$	384.021 [°C]
Comb all	$L1$	3.249e+04 [°C]
Comb 5th	$L1$	3.407e+03 [°C]



# Appendix C

## Temperature profiles

### C.1 Case 1a

Temperature profiles of the distillation column in the different active constraint regions.

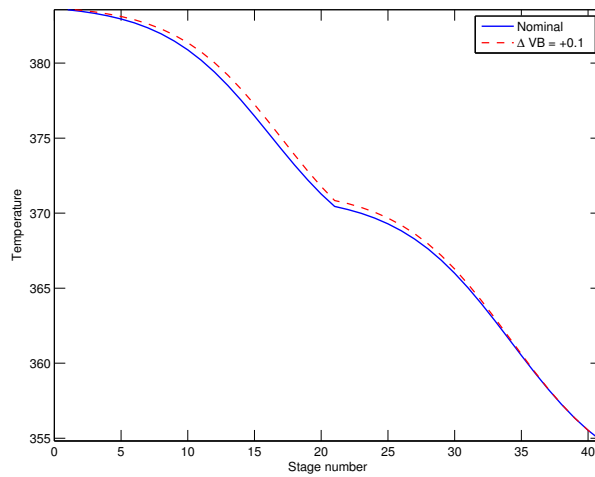
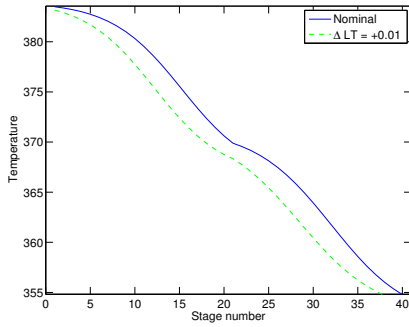


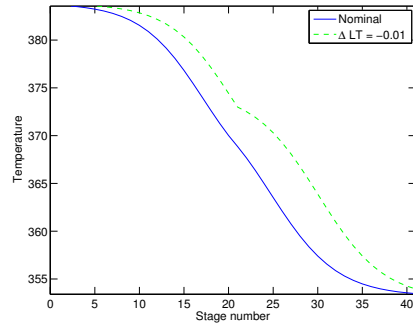
Figure C.1: Temperatureprofile of region I.

## C.2 Case 1b

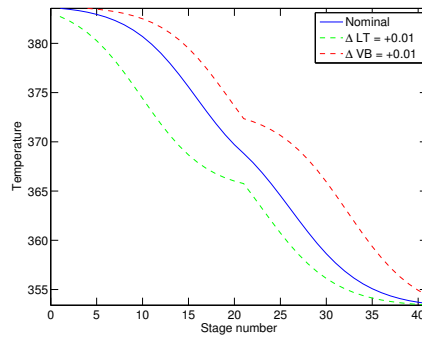
Temperature profiles of the distillation column for the different regions.



(a) Region I



(b) Region IV

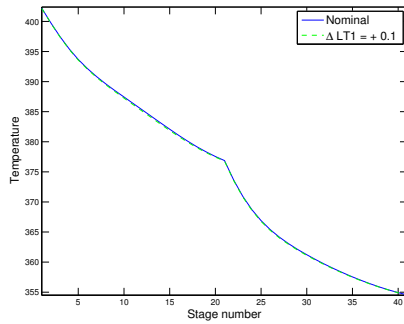


(c) Region V

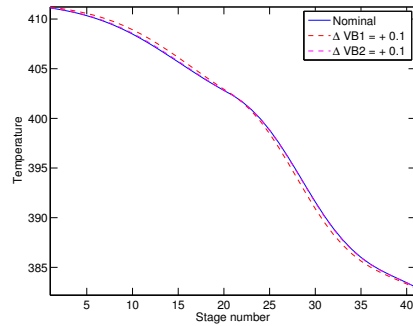
Figure C.2: Temperature profiles for case study 1b.

## C.3 Case 2

Temperature profiles of the two distillation columns in sequence for the different regions.

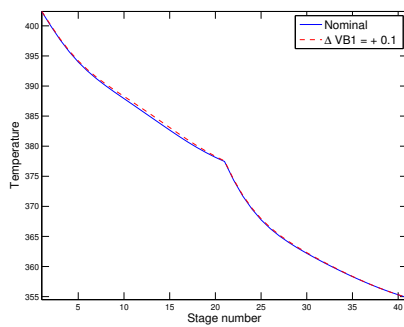


(a) Column 1

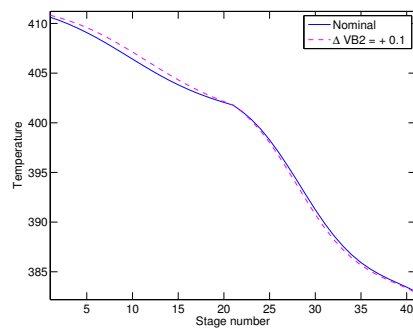


(b) Column 2

Figure C.3: Temperature profiles for region I.



(a) Column 1



(b) Column 2

Figure C.4: Temperature profiles for region II.

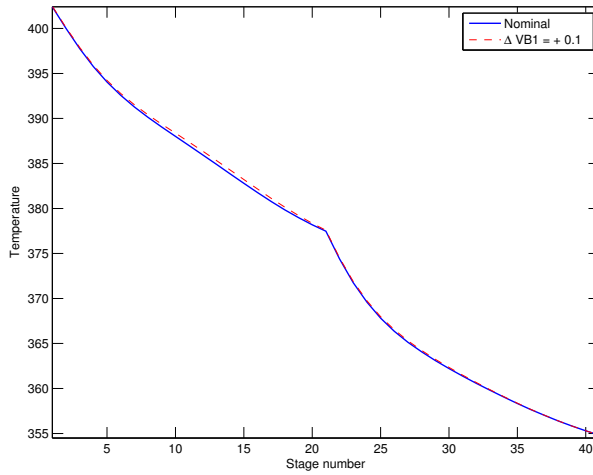
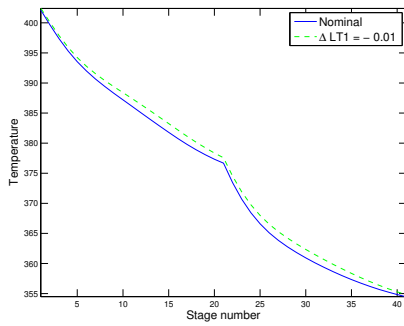
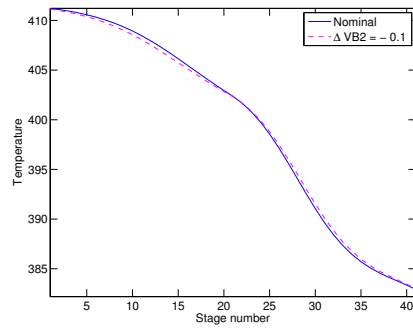


Figure C.5: Temperature profile of region III.



(a) Column 1



(b) Column 2

Figure C.6: Temperature profiles for region IV.

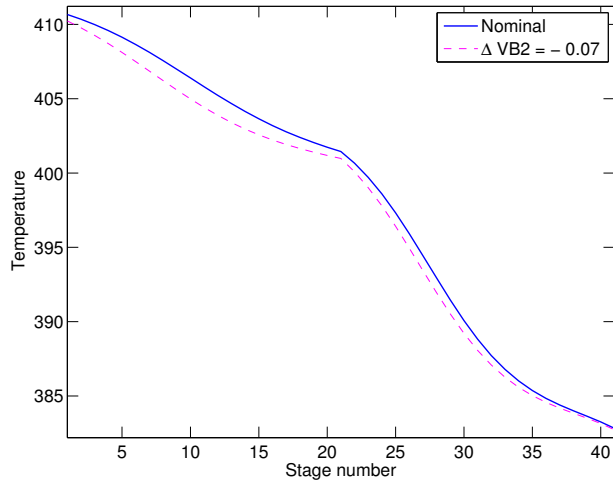


Figure C.7: Temperatureprofile of region V.

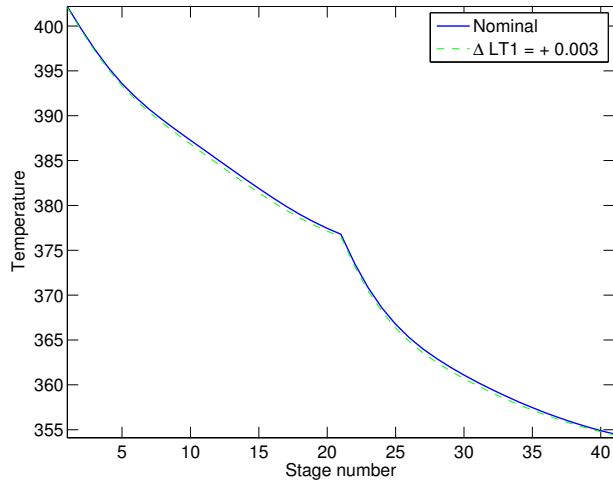


Figure C.8: Temperatureprofile of region VII.



# Appendix D

## AMPL code

The AMPL code for the run file and distillation model of case studies 1a and 1b are shown in below.

```
#####
# Optimization of a distillation column with
# parameters Energy price, pV, and feed rate, F.
#####

#-----
# Setting parameters as variables
#-----

var F ;          # feed
var zF ;         # feed composition
var qF ;         # feed liquid composition
var pV ;        # price vapor($)

#-----
# PARAMETERS
#-----

param NT, := 41 ;      # number of stages including reboiler
param NF, := 21 ;     # location of of feed stage (counted from the bottom)

### P-Controllers for control of reboiler and condenser hold up

param KcB, := 10 ;    # controller gain reboiler
param KcD, := 10 ;    # controller gain condenser
param MDs, := 0.5 ;  # nominal holdup condenser
param MBs, := 0.5 ;  # nominal holdup reboiler
param Ds, := 0.5 ;   # nominal flow condenser
param Bs, := 0.5 ;   # nominal flow reboiler

param alpha, := 1.5 ; # relative volatility
```

```

param M0, := 0.5 ;                #nominal liquid holdups

### Data for linearized liquid flow dynamics
# (does not apply to reboiler or condenser)

param tau1, := 0.063;  # time constant for liquid dynamics (min)
param F0, := 1 ;      # nominal feed rate (kmol/min)
param qF0, := 1 ;    # nominal fraction of liquid
param L0, := 2.70629 ; # nominal reflux flow (from steady-state data)
param L0b, >= 0 ;    # nominal liquid flow below flow (kmol/min)
param lambda, := 0 ; # effect of vapor flow on liquid flow ("K2-effect")
param V0, := 3.20629 ; # nominal vapor flow
param V0t, >= 0 ; # nominal vapor flow

### Define prices

param pF, := 1 ;                # feed price ($)
param pB, := 1 ;                # bottoms price ($)
param pD, := 2 ;                # price distillate ($)

#-----
# VARIABLES
#-----
var LT >= 0.1 <= 10 := 2.76969 ;
var VB >= 0.1 <= 10 := 3.39585 ;

var L {2..NT} >= 0 ;
var V {1..NT-1} >= 0 ;

var D >= 0 ;          # distillate flow
var B >= 0 ;          # bottoms flow

var MB >= 0 ;        # actual reboiler holdup
var MD >= 0 ;        # actual condenser holdup

var x {1..2*NT} >= 0 ;
var y {1..NT-1} >= 0 ;

#-----
# Initial values for stages/holdup and distillate and bottom flow
#-----
for {i in 1..2*NT}
let x[i] := 0.5 ; # initial values for composition in the stages

let L0b := L0 + qF0*F0 ;
let V0t := V0 + (1 - qF0)*F0 ;

#-----
# CONSTRAINTS

```



```

#-----

### Control liquid level in reboiler and condenser
const1:
    MB = x[NT+1] ;
const2:
    MD = x[2*NT] ;
const3:
    B = Bs + (MB - MBs)*KcB ;
const4:
    D = Ds + (MD - MDs)*KcD ;

### Model
const5 {i in 1..NT-1}:
    y[i] = alpha*x[i]/(1 + (alpha-1)*x[i]); # vapor-liquid equilibria

const6 {i in 1..NF-1}:
    V[i] = VB ; # vapor flow below feed

const7 {i in NF..NT-1}:
    V[i] = VB + (1-qF)*F ; # vapor flow above feed

const8 {i in 2..NF}:
    # liquid flow below feed
    L[i] = LOb + (x[i+NT] - M0)/tau1 + lambda*(V[i-1] - V0) ;

const9 {i in NF+1..NT-1}:
    # liquid flow above feed
    L[i] = LO + (x[i+NT] - M0)/tau1 + lambda*(V[i-1] - V0t) ;

const10:
    L[NT] = LT ; # liquid flow condenser

const11 {i in 2..NF-1}:
    L[i+1] - L[i] + V[i-1] - V[i] = 0 ; # dMdt below feed

const12 {i in 2..NF-1}:
    L[i+1]*x[i+1] - L[i]*x[i] + V[i-1]*y[i-1]
    - V[i]*y[i] = 0 ; # dMxdt above feed

const13 {i in NF+1..NT-1}:
    L[i+1] - L[i] + V[i-1] - V[i] = 0 ; # dMdt above feed

const14 {i in NF+1..NT-1}:
    L[i+1]*x[i+1] - L[i]*x[i] + V[i-1]*y[i-1]
    - V[i]*y[i] = 0 ; # dMxdt above feed

const15:
    L[2] - V[1] - B = 0 ; # dMdt reboiler

const16:

```

```

    L[2]*x[2] - V[1]*y[1] - B*x[1] = 0 ;          # dMxdt reboiler

const17:
    L[NF+1] - L[NF] + V[NF-1] - V[NF] + F = 0 ; # dMdt feed

const18:
    L[NF+1]*x[NF+1] - L[NF]*x[NF] + V[NF-1]*y[NF-1]
    - V[NF]*y[NF] + F*zF = 0 ;          # dMxdt feed

const19:
    V[NT-1] - LT - D = 0 ;              # dMdt condenser

const20:
    V[NT-1]*y[NT-1] - LT*x[NT] - D*x[NT] = 0 ;# dMxdt condenser

### Inequality constraints
const21:
    1 - x[1] >= 0.99 ;                  # fraction of heavy comp in bottom

const22:
    x[NT] >= 0.95 ; # fraction of light comp in distillate

const23:
    VB <= 4.008 ;                       # max vapor flow

### Initial constraints for parameters
constF: F = nominal_F ;
constpV: pV = nominal_pV ;
constzF: zF = nominal_zF ;
constqF: qF = nominal_qF ;

#-----
# OBJECTIVE FUNCTION
#-----
minimize cost: pF*F + pV*VB - pB*B - pD*D ;

```

The AMPL code for the run file and distillation model of case study 2 are shown below.

```
#####  
# RUN FILE #  
#####  
  
reset ;  
  
#-----  
# Set parameters  
#-----  
  
param nominal_F := 1.35 ;  
param d1_perturbed_F := 1.35 ;  
param d2_perturbed_F := 1.35 ;  
param d3_perturbed_F := 1.35 ;  
  
param nominal_pV := 0.03 ;  
param d1_perturbed_pV := 0.03 ;  
param d2_perturbed_pV := 0.03 ;  
param d3_perturbed_pV := 0.03 ;  
  
# param nominal_zF := 0.5 ;  
# param d1_perturbed_zF := 0.5 ;  
# param d2_perturbed_zF := 0.5 ;  
# param d3_perturbed_zF := 0.5 ;  
# param d4_perturbed_zF := 0.5 ;  
  
param nominal_qF := 1 ;  
param d1_perturbed_qF := 1 ;  
param d2_perturbed_qF := 1 ;  
param d3_perturbed_qF := 1 ;  
  
#-----  
# Declare suffixes for sIopt code  
#-----  
  
# enumerate parameters that will be perturbed  
suffix sens_state_0, IN ;  
  
# enumerate parameters that will be perturbed and also indicate the  
# order for parameters at the perturbed value  
suffix sens_state_1, IN ;
```

```
# communicates the values for the perturbed parameters
suffix sens_state_value_1, IN ;

# holds the updated values variables as well as the constraint
# multiplier values computed
suffix sens_sol_state_1, OUT ;

suffix sens_state_2, IN ;
suffix sens_state_value_2, IN ;
suffix sens_sol_state_2, OUT ;

suffix sens_state_3, IN ;
suffix sens_state_value_3, IN ;
suffix sens_sol_state_3, OUT ;

# flag that indicates that a constraint is artificial
suffix sens_init_constr, IN ;

# Used for sIopt to compute the Hessian
suffix red_hessian, IN ;

#-----
# Options
#-----
option solver "/Users/Roald/ipopt_sens";
option show_stats 1 ;

option ipopt_options 'max_iter=1000';

### turn presolve off
option presolve 0;

### hessian
option ipopt_options 'compute_red_hessian yes';

### load model
model twodist.mod ;

#-----
# sIopt data
#-----

### feed
let F.sens_state_0 := 1 ;
let F.sens_state_1 := 1 ;
let F.sens_state_value_1 := d1_perturbed_F ;
```

---

```

let F.sens_state_2 := 1;
let F.sens_state_value_2 := d2_perturbed_F ;
let F.sens_state_3 := 1;
let F.sens_state_value_3 := d3_perturbed_F ;

### energy price
let pV.sens_state_0 := 2 ;
let pV.sens_state_1 := 2 ;
let pV.sens_state_value_1 := d1_perturbed_pV ;
let pV.sens_state_2 := 2 ;
let pV.sens_state_value_2 := d2_perturbed_pV ;
let pV.sens_state_3 := 2;
let pV.sens_state_value_3 := d3_perturbed_pV ;

### feed liquid fraction
let qF.sens_state_0 := 3 ;
let qF.sens_state_1 := 3 ;
let qF.sens_state_value_1 := d1_perturbed_qF ;
let qF.sens_state_2 := 3 ;
let qF.sens_state_value_2 := d2_perturbed_qF ;
let qF.sens_state_3 := 3;
let qF.sens_state_value_3 := d3_perturbed_qF ;

let constF.sens_init_constr := 1 ;
let constpV.sens_init_constr := 2 ;
let constqF.sens_init_constr := 3 ;

let LT1.red_hessian := 1 ;
let VB1.red_hessian := 2 ;
let LT2.red_hessian := 3 ;
let VB2.red_hessian := 4 ;

#####
# Solve
#####
solve ;

#####
# Print
#####
print "";
print "Nominal Solution:";
display VB1, VB2, F, pV, qF, x1[NT,1], x2[NT,2], 1-(x2[1,1]+x2[1,2]);

```

```
print "F Perturbed Solution with sIPOPT:";
display LT1.sens_sol_state_1, LT2.sens_sol_state_1,
VB1.sens_sol_state_1, VB2.sens_sol_state_1;

display F.sens_sol_state_1, pV.sens_sol_state_1,
qF.sens_sol_state_1;

display x1.sens_sol_state_1, x2.sens_sol_state_1;

print "pV Perturbed Solution with sIPOPT:";
display LT1.sens_sol_state_2, LT2.sens_sol_state_2,
VB1.sens_sol_state_2, VB2.sens_sol_state_2;

display F.sens_sol_state_2, pV.sens_sol_state_2,
qF.sens_sol_state_2;

display x1.sens_sol_state_2, x2.sens_sol_state_2;

print "qF Perturbed Solution with sIPOPT:";
display LT1.sens_sol_state_3, LT2.sens_sol_state_3,
VB1.sens_sol_state_3,
VB2.sens_sol_state_3;

display F.sens_sol_state_3, pV.sens_sol_state_3, qF.sens_sol_state_3;

display x1.sens_sol_state_3, x2.sens_sol_state_3;
```

```

#####
# The distillation model #
#####

### Two columns in series
### Three components: A (light), B and C (heavy).
### Based on Column A. Steady state model.

### made by Roald Brck Leer

#-----
# Setting parameters as variables
#-----

# Disturbances
var F >= 0.1 ;                #feed
var qF ;                      #liquid fraction in feed
var pV ;                      #energy price

#-----
# Parameters
#-----

param NT := 41 ;              #stages
param NC := 3 ;              #number of components
param NF := 21 ;            #feed enter at stage 21

### Relative volatility, alpha(A/B) alpha(B/C)
param alpha {1..2} ;
let alpha[1] := 2.0 ;
let alpha[2] := 1.5 ;

### Diagonal matrix of relative volatilities
param m_alpha {1..2,1..2} ;
for {i in 1..2, j in 1..2}
let m_alpha[i,j] := 0 ;
for {i in 1..2}
let m_alpha[i,i] := alpha[i] ;

### Parameters for Franci's Weir Formula  $L(i) = K \cdot Mow(i)^{1.5}$ 
param Kuf := 21.65032 ;      # constant above feed
param Kbf := 29.65032 ;      # constant below feed
param Muw := 0.25 ;         # liquid holdup under weir (kmol)

### P-Controllers for control of reboiler and condenser hold up
param KcB, := 10 ;          # controller gain reboiler
param KcD, := 10 ;          # controller gain condenser
param MDs, := 0.5 ;        # nominal holdup condenser
param MBs, := 0.5 ;        # nominal holdup reboiler
param Ds, := 0.5 ;         # nominal flow condenser

```

```

param Bs, := 0.5 ;                # nominal flow reboiler

param M0, := 0.5 ;                #nominal liquid holdups

### Define prices
param pF, := 1 ;                  # feed price ($)
param pA, := 1 ;                  # light comp price ($)
param pB, := 2 ;                  # medium comp price ($)
param pC, := 1 ;                  # heavy comp price ($)

param zF {1..1,1..3} ;           # feed composition
let zF[1,1] := 0.4 ;
let zF[1,2] := 0.2 ;
let zF[1,3] := 0.4 ;

#-----
# Variables
#-----

### FIRST COLUMN

var LT1 >= 0 <= 10 := 3.43656 ;
var VB1 >= 0 <= 10 := 4.008 ;

### comp frac liquid and vap
var y1 {i in 1..NT-1, j in 1..2} >= 0 := 0.3 ; # vapor comp
var x1 {i in 1..NT, j in 1..2} >= 0 := 0.4 ; # liquid comp

var M1 {i in 1..NT} >= 0 := 0.5 ;                # holdup

var V1 {1..NT-1} >= 0 := 1 ;                    # vapor flow
var L1 {2..NT} >= 0 := 1 ;                      # liquid flow

var D1 >= 0 := 0.57 ;                          # distillate flow
var B1 >= 0 := 0.83 ;                          # bottoms flow

# VLE equation split
var y_1_1 {i in 1..NT-1, j in 1..2} >= 0 := 0.2 ;
var y_1_2 {i in 1..NT-1, j in 1..2} >= 0 := 0.7 ;

### SECOND COLUMN

var LT2 >= 0 <= 10 := 2.13827 ;
var VB2 >= 0 <= 10 := 2.40367 ;

### comp frac liquid and gas
var y2 {i in 1..NT-1, j in 1..2} >= 0 := 0.5 ; # vapor comp
var x2 {i in 1..NT, j in 1..2} >= 0 := 0.4 ; # liquid comp

var M2 {i in 1..NT} >= 0 := 0.5 ;                # holdup

```



```

var V2 {1..NT-1} >= 0 :=1;           # vapor flow
var L2 {2..NT} >= 0 :=1;           # liquid flow

var D2 >= 0 := 0.26 ;              # distillate flow
var B2 >= 0 := 0.56 ;              # bottoms flow

# VLE equation split
var y_2_1 {i in 1..NT-1, j in 1..2} := 0.3 ;
var y_2_2 {i in 1..NT-1, j in 1..2} := 0.8 ;

#-----
# Model/Constraints 1
#-----

### VLE equation split
const1 {i in 1..NT-1, j in 1..2} :
    y_1_1[i,j] = x1[i,j]*m_alpha[j,j] ;

const2 {i in 1..NT-1, j in 1..2}:
    y_1_2[i,j] = ((x1[i,1]*(alpha[1]-1)+x1[i,2]*(alpha[2]-1))+1) ;

### Vapour-liquid equilibria (multicomponent ideal VLE,
# Stichlmair-Fair, 'Distillation', p. 36, 1998)
const3 {i in 1..NT-1, j in 1..2}:
    y1[i,j] = y_1_1[i,j]/y_1_2[i,j] ;

### Vapor flows assuming constant molar flows
const4 {i in 1..NF-1}:
    V1[i] = VB1 ;          # vapor flow below feed

const5 {i in NF..NT-1}:
    V1[i] = VB1 + (1-qF)*F ;      # vapor flow above feed

### Liquid flows are given by Franci's Weir Formula  $L(i)=K*Mow(i)^{1.5}$ 
# Liquid flow L(i) dependent only on the holdup over the weir Mow(i)
#M(i)= Mow(i) + Muw(i) (Total holdup = holdup over weir +
#holdup below weir)

const6 {i in 2..NF}:
    L1[i] = Kbf*(M1[i] - Muw)^1.5 ; # Liquid flow below feed

const7 {i in NF+1..NT-1}:
    L1[i] = Kuf*(M1[i] - Muw)^1.5 ;# Liquid flows above feed

const8:
    L1[NT] = LT1;          # Condenser's liquid flow

```

```

### Distillate and bottom
const9:
    B1 = Bs + (M1[1] - MBs)*KcB ;

const10:
    D1 = Ds + (M1[NT] - MDs)*KcD ;

### Material balances for total holdup and component holdup
const11 {i in 2..NF-1}:
    L1[i+1] - L1[i] + V1[i-1] - V1[i] = 0 ; # dM below feed

const12 {i in NF+1..NT-1}:
    L1[i+1] - L1[i] + V1[i-1] - V1[i] = 0 ; # dM above feed

const13 {i in 2..NF-1, j in 1..2}:
    L1[i+1]*x1[i+1,j] - L1[i]*x1[i,j] + V1[i-1]*y1[i-1,j]
    - V1[i]*y1[i,j] = 0 ;

const14 {i in NF+1..NT-1, j in 1..2}:
    L1[i+1]*x1[i+1,j] - L1[i]*x1[i,j] + V1[i-1]*y1[i-1,j]
    - V1[i]*y1[i,j] = 0 ;

### Correction for feed at the feed stage: The feed is assumed to
#be mixed into the feed stage
const15:
    L1[NF+1] - L1[NF] + V1[NF-1] - V1[NF] + F = 0 ;

const16:
    L1[NF+1]*x1[NF+1,1] - L1[NF]*x1[NF,1] + V1[NF-1]*y1[NF-1,1]
    - V1[NF]*y1[NF,1] + F*zF[1,1] = 0 ;

const17:
    L1[NF+1]*x1[NF+1,2] - L1[NF]*x1[NF,2] + V1[NF-1]*y1[NF-1,2]
    - V1[NF]*y1[NF,2] + F*zF[1,2] = 0 ;

### Reboiler (assumed to be an equilibrium stage)
const18:
    L1[2] - V1[1] - B1 = 0 ;

const19 {j in 1..2}:
    L1[2]*x1[2,j] - V1[1]*y1[1,j] - B1*x1[1,j] = 0 ;

### Total condenser (no equilibrium stage)
const20:
    V1[NT-1] - LT1 - D1 = 0 ;

const21 {j in 1..2}:
    V1[NT-1]*y1[NT-1,j] - L1[NT]*x1[NT,j] - D1*x1[NT,j] = 0 ;

```

```

#-----
# Model/Constraints 2
#-----

### VLE equation split
const21 {i in 1..NT-1, j in 1..2} :
    y_2_1[i,j] = x2[i,j]*m_alpha[j,j] ;

const22 {i in 1..NT-1, j in 1..2}:
    y_2_2[i,j] = ((x2[i,1]*(alpha[1]-1)+x2[i,2]*(alpha[2]-1))+1) ;

### Vapour-liquid equilibria (multicomponent ideal VLE,
# Stichlmair-Fair, 'Distillation', p. 36, 1998)
const23 {i in 1..NT-1, j in 1..2}:
    y2[i,j] = y_2_1[i,j]/y_2_2[i,j] ;

### Vapor flows assuming constant molar flows
const24 {i in 1..NF-1}:
    V2[i] = VB2 ;          # vapor flow below feed

const25 {i in NF..NT-1}:
    V2[i] = VB2 ;          # vapor flow above

const26 {i in 2..NF}:
    L2[i] = Kbf*(M2[i] - Muw)^1.5 ; # Liquid flow below feed

const27 {i in NF+1..NT-1}:
    L2[i] = Kuf*(M2[i] - Muw)^1.5 ; # Liquid flow above feed

const28:
    L2[NT] = LT2;          # Condenser's liquid flow

const29:
    B2 = Bs + (M2[1] - MBs)*KcB ;

const30:
    D2 = Ds + (M2[NT] - MDs)*KcD ;

### Material balances for total holdup and component holdup

const31 {i in 2..NF-1}:
    L2[i+1] - L2[i] + V2[i-1] - V2[i] = 0 ; # dM below feed

const32 {i in NF+1..NT-1}:
    L2[i+1] - L2[i] + V2[i-1] - V2[i] = 0 ; # dM above feed

```

```

const33 {i in 2..NF-1, j in 1..2}:          # dMxdt below feed
    L2[i+1]*x2[i+1,j] - L2[i]*x2[i,j] + V2[i-1]*y2[i-1,j]
    - V2[i]*y2[i,j] = 0 ;

const34 {i in NF+1..NT-1, j in 1..2}:      # dMxdt above feed
    L2[i+1]*x2[i+1,j] - L2[i]*x2[i,j] + V2[i-1]*y2[i-1,j]
    - V2[i]*y2[i,j] = 0 ;

### Correction for feed at the feed stage: The feed is assumed to be
# mixed into the feed stage
const35:
    L2[NF+1] - L2[NF] + V2[NF-1] - V2[NF] + B1 = 0 ;

const36:
    2[NF+1]*x2[NF+1,1] - L2[NF]*x2[NF,1] + V2[NF-1]*y2[NF-1,1]
    - V2[NF]*y2[NF,1] + B1*x1[1,1] = 0 ;

const37:
    L2[NF+1]*x2[NF+1,2] - L2[NF]*x2[NF,2] + V2[NF-1]*y2[NF-1,2]
    - V2[NF]*y2[NF,2] + B1*x1[1,2] = 0 ;

### Reboiler (assumed to be an equilibrium stage)
const38:
    L2[2] - V2[1] - B2 = 0 ;

const39 {i in 1..2}:
    L2[2]*x2[2,i] - V2[1]*y2[1,i] - B2*x2[1,i] = 0 ;

### Total condenser (no equilibrium stage)
const40:
    V2[NT-1] - LT2 - D2 = 0 ;

const41 {i in 1..2}:
    V2[NT-1]*y2[NT-1,i] - L2[NT]*x2[NT,i] - D2*x2[NT,i] = 0 ;

### Inequality constraints
const42:
    x1[NT,1] >= 0.95 ;                      # xA

const43:
    x2[NT,2] == 0.95 ;                      # xB

const44:
    1 - (x2[1,1]+x2[1,2]) >= 0.95 ;        # xC

const45:
    VB1 <= 4.008 ;                          # max boilup column 1

```

---

```
const46:
    VB2 <= 2.405 ;                # max boilup column 2

### Initial constraints for parameters
constF: F = nominal_F ;
constpV: pV = nominal_pV ;
# constzF: zF = nominal_zF ;
constqF: qF = nominal_qF ;

#-----
# OBJECTIVE FUNCTION
#-----
minimize cost: pF*F + pV*(VB1 + VB2) - pA*D1 - pB*D2 - pC*B2 ;
```