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Control strategies for divided wall (Petlyuk) columns

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Summary

Based on economic plantwide control procedure, all possible modes of optimal operation for the three-product divided wall column has been presented.

The optimal operation of one of these modes with fixed energy and unconstrained product purities has been studied. The objective cost function was to minimize the sum of impurities in all three product streams. None of the product purity compositions was active and there were three unconstrained degrees of freedom. These unconstrained degrees of freedom were used for self-optimizing control.

Since the objective cost function was to minimize the sum of impurities therefore instead of compositions temperatures on all stages were assumed to be better choice as candidate controlled variables.

Selection of controlled variables is very important task in the system with self-optimizing control configuration for optimal operation. In this study, pseudo-steady-state loss evaluations method based on linearized model was used to prescreen the candidate controlled variables. The branch and bound method was used to get best sets of measurement combinations based on the largest value of minimum singular value. Also, bi-directional branch and bound method using average loss criterion was used to get best sets of measurement combinations. Further to evaluate these measurement combinations, exact local method (minimum loss method) was used. The exact local method was used to calculate the measurement combination matrices H and based on these values average and worst-case loss in each case was calculated. The calculation of average loss based on the exact local method gave best sets of controlled variables. The average loss was also calculated using exact local method for all combination of measurement with and without measurement noise. The loss with all combinations of measurement was less than that for three combinations of measurement.

The loss evaluation for all the combination matrices H was done with larger disturbances on the non-linear model of the column at steady-state. The three

combinations of measurement approved the results obtained from steady-state loss analysis whereas all combinations of measurement gave unacceptable loss.

Finally for one of these best sets the control configuration was also proposed. The control configuration seemed working pretty well for self-optimizing control giving acceptable loss after disturbances.

Preface

The Master Thesis work has been done as a part of compulsory course work during the Master in Chemical Engineering Program at the Norwegian University of Science and Technology (NTNU). The subject of the thesis falls in the domain of Process System Engineering which also happened to be the field of my specialization in Chemical Engineering. The topic of the thesis – “Control strategies for divided-wall (Petlyuk) column” was chosen in the context of the following theme:

“Divided wall column has been proved to be superior in terms of energy, space as well as capital saving over the conventional distillation column in theory as well as in practice. While there are hundred thousands of conventional columns in Chemical plants around the world the number of such columns is relatively very few (approximately 140). The reason behind limited implementation of such columns is the complexity in design and control.”

“The challenges associated with the control problem actually became the interest of this work and the work was started to address the problems related to the control structure design of the three-product divided wall column. The title itself was very subjective therefore after a few brain-storming sessions on various possible unique cases of operation the objective and the periphery of the task were decided.”

First and foremost, I would like to express my whole hearted appreciation and gratitude to my supervisor Professor Sigurd Skogestad. His extraordinary high level of knowledge was inspiring and working under his supervision was rare achievement. I had my undergraduate degree in Mechanical Engineering and I had started working in a completely new field. But things turned out to be much easier because of his effective supervision and guidance. I will be forever grateful to him for all the knowledge I have gained while working with him.

I am grateful to Ivar J. Halvorsen for providing me with valuable suggestions on my work and answering my conceptual queries related to the divided wall columns. I am also thankful to Deepatanshu Dwivedi for introducing me to the core program as an initial backup to move on with the thesis work. Special thanks would go to Moritz Gleinser, previous exchange student at NTNU for all the discussion via email without having met me even once.

While working on my thesis, there were many moments when I felt the need to cross-check the authenticity of my approach towards solving problems. Thanks to people at process control group- Johannes Jäschke, Vladimoros L. Minasidisimir, Tor Anders Marvik for answering my queries and all those informative discussions.

It would be too formal to thank my husband M. Shamsuzzoha on this piece of paper but he definitely needs the acknowledgment for supporting my study and stay in Norway. With his encouragement and support, I came back and finished my study. Above all, this thesis is dedicated to my dearest daughter Haadiya Shams because some of the quality time which was supposed to be spent with her was diverted to my study.

Declaration of Compliance

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

Author _____

Date _____

TABLE OF CONTENTS

Summary	i
Preface	iii
List of figures	ix
List of Tables	xi
List of Symbols and Abbreviations	xii
CHAPTER 1 Introduction	1
1.1 Motivation and Literature Review	1
1.1 Scope of Thesis Work.....	3
1.2 Thesis Overview	4
1.3 Publications.....	5
CHAPTER 2 Distillation Fundamentals	6
2.1 Distillation	6
2.1.1 Relative Volatility.....	6
2.1.2 Separation Factor	7
2.1.3 Assumptions.....	7
2.1.3.1 Constant Relative Volatilities	7
2.1.3.2 Equilibrium on Stages	8
2.1.3.3 Constant Molar Flows:	9
2.1.3.4 Estimation of Temperature from Composition and Boiling points	9
2.1.3.5 Linearized Liquid Flow Dynamics	9
2.2 The column in Sequence.....	10

2.2.1	Direct Sequence	10
2.2.2	Indirect Column Sequence	11
2.2.3	Thermodynamic Implementation of Three-Product Petlyuk Column	13
CHAPTER 3 Optimal Selection of Controlled Variables		15
3.1	Plantwide Control Procedure	15
3.1.1	Top- Down Analysis (Economics).....	17
3.1.2	Bottom-Up Analysis (Stabilization)	20
3.2	Self-optimizing Control	20
3.2.1	Methods for Loss Evaluation	22
3.2.1.1	Variable and Notations	23
3.2.1.2	Cost Function.....	23
3.2.1.3	Assumptions	24
3.2.2	Re-defining the Minimum Loss method	24
3.2.2.1	Solution to Minimum Loss Problem (Exact Local Method)	25
3.2.2.2	The Maximum Minimum Singular Rule	27
3.2.2.3	Null Space Method	29
3.2.3	Loss Evaluation form Dynamic Simulations (Validation).....	29
3.2.3.1	Controller Tuning	29
3.2.3.2	First Order Process	30
3.2.3.3	The Integrating Process	31
3.2.3.4	The sequential Design of Decentralized Control.....	32
CHAPTER 4 Control Strategies for Divided Wall Column		33
4.1	Process Description and Model	33
4.2	Plantwide Control Procedure for the Column.....	36
4.2.1	Define the Objective Function and the Constraints (DWC)	36

4.2.2	Optimization (Offline-Analysis, DWC).....	38
4.2.3	Implementation of the Optimal Operation (DWC).....	39
4.2.4	Where to Set the Production Rate (DWC).....	40
4.2.5	Regulatory Control Layer (DWC)	40
4.2.6	Selection of Controlled Variables and Loss –evaluation (DWC).....	40
CHAPTER 5 Simulation Procedure.....		42
5.1	Initialize the Steady-State Simulation.....	42
5.1.1	Defining the Design Conditions.....	42
5.2	Optimization	44
5.3	Evaluation of Loss from Steady-state Linearized Model	44
5.4	Evaluation of Loss from Non-linear Model.....	46
5.5	Evaluation of Loss from Dynamic Model	46
CHAPTER 6 Results and Discussion		50
6.1	Initial Steady-State Simulation	50
6.1.1	Defining the design conditions	50
6.2	The Nominal Values from Optimization	52
6.3	Re-optimized values with disturbances	55
6.4	Loss Evaluations using Pseudo/Steady-state Linearized Model.....	56
6.5	Results from Maximum Minimum Singular Rule	56
6.5.1	Optimal Sensitivities.....	56
6.5.2	Scaled Gain	60
6.6	Loss Evaluation using H matrix (Local Methods).....	62
6.6.1	Loss Evaluation with three Measurements	62
6.6.2	Loss Evaluation (Exact Local Method)	65
6.6.3	Loss Evaluation (Null Space Method).....	66

6.7	Loss Evaluation from Non-linear Model	66
6.8	Results from dynamic simulation	71
CHAPTER 7 Conclusion and Further Work.....		75
7.1	Conclusion	75
7.2	Further Work.....	76
Bibliography		78
APPENDIX A Matlab Codes		83
	Matlab Codes (Steady-state Simulation)	83
	Matlab Codes for Self-optimizing Control	93
	Mtalab Codes for Dynamic Simulations.....	116

List of figures

Figure 2-1: Direct column sequence for the separation of three products.....	10
Figure 2-2: Indirect column sequence for the separation of three products	11
Figure 2-3: (a) Thermodynamically equivalent implementations of three-product DWC (b) DWC implementation	13
Figure 3-1: Typical control hierarchy in a chemical plant (Larsson and Skogestad)	16
Figure 3-2: Feedback implementation of optimal operation with separate layers for optimization and control, (Kassidas, Patry and Marlin 2000) and (Engell 2007)	19
Figure 3-3: Cost function as a function of disturbance d & d^* and inputs u , (Yelchuru 2012)	21
Figure 3-4: The feed-back control diagram for self-optimizing control, (Yelchuru 2012)	22
Figure 3-5: Open loop step -response for first order process model (S. Skogestad 2013)	31
Figure 4-1: The schematic diagram of the three-product divided wall column.....	34
Figure 6-1: V_{\min} diagrams for two different compositions of feed with relative volatilities, $\alpha = [4.2 \ 2.1 \ 1]$	51
Figure 6-2: Optimal composition profiles in the prefractionator and the main column respectively of the three-product divided wall column.....	54
Figure 6-3: Optimal temperature profile in the three-product divided wall column	54
Figure 6-4: Optimal-sensitivity of output temperatures with respect to the boilup.....	57
Figure 6-5: Optimal-sensitivity of output temperatures with respect to the feed	58
Figure 6-6: Optimal sensitivity of output temperatures with respect to composition of A in the feed.....	58
Figure 6-7: Optimal-sensitivity of output temperatures with respect to composition of B in the feed	59

Figure 6-8: Optimal-sensitivity of output temperatures with respect to the vapor split ratio	59
Figure 6-9: Scaled gains in the prefractionator and the main column for unconstrained degrees of freedom	60
Figure 6-10: The loss obtained from the non-linear model due to disturbance in feed flow rate for self-optimizing control by keeping three temperatures constant	68
Figure 6-11 : The loss obtained from the non-linear model due to disturbance in feed for self-optimizing control by null space method	69
Figure 6-12 : The loss obtained from the non-linear model due to disturbance in feed for self-optimizing control by exact local method for all combination of measurements.....	70
Figure 6-13: Self-optimizing control configuration (keeping three temperatures at their nominal setpoints using unconstrained degrees of freedom).....	73

List of Tables

Table 4-1: Process data for the three-product divided wall column	35
Table 4-2: Possible modes of operation for the three product divided wall column based on the active constraints.....	38
Table 5-1: SIMC tuning parameters used in the self-optimizing control structure	49
Table 6-1: Input values used for initial steady-state simulation with 12 stages in each section	52
Table 6-2: Compositions at steady-state in the main column and the prefractionator of the column	52
Table 6-3: The input values at the nominal conditions for DWC	53
Table 6-4: Product compositions in the main column and the prefractionator of DWC .	53
Table 6-5: The re-optimized cost with respect to expected future disturbances.....	55
Table 6-6: Ten best sets of temperature as candidate controlled variables based on maximum minimum singular value rule	62
Table 6-7: Average loss and worst-case loss for 10 best sets of measurements (here, $n_y = n_u$) using minimum loss method.....	63
Table 6-8: Average loss and worst-case loss for ten best sets of measurements (here, $n_y = n_u$) using bidirectional branch and bound method, (Kariwala, Cao and Janardhanan 2008)	64
Table 6-9: The steady-state RGA for the selected controlled variables	72
Table 6-10: The product purity compositions and percentage loss for +10% change in disturbances from nominal.....	73
Table 6-11: The product purity compositions and percentage loss for -10% change in disturbances from nominal.....	74

List of Symbols and Abbreviations

Symbols	Description [Units]
α	Relative volatility between two components
p	Pure component vapor pressure
x	Mole fraction in liquid phase [kmol/kmol]
γ	Activity coefficient in the liquid phase
y	Mole fraction in vapor phase [kmol/kmol]
S	Separation factor
K	Equilibrium constant
τ_1	Dominant lag time constant of the process [min]
L_n	Liquid flow rate on n^{th} stage [kmol/min]
V_n	Vapor flow rate on n^{th} stage [kmol/min]
M_i	Liquid holdup on i^{th} stage [kmol/min]
λ	Time constant
u	Input variables/manipulated variables
d	Disturbance variables
R^{n_x}	Set of state variables
R^{n_d}	Set of disturbance variables
T	Temperature
G'	Scaled steady-state gain
c_s	Controlled variables setpoints
J	Cost function [[\$/min]
H	Measurement combination matrix
n^y	Measurement noise
L_{wc}	Worst case loss
u_{opt}	Optimal values of input
d^*	Optimal values of disturbances
G^y	Process gain matrix
C_{opt}	Optimal values of controlled variables
F	Feed flow rate [kmol/min]

$[z_A z_B z_C]$	Mole fraction of components A, B and C respectively in feed
V_{max}	Maximum boilup [kmol/min]
R_v	Vapor split ratio
V_{min}	Minimum boilup [kmol/min]
L	Reflux flow rate [kmol/min]
V	Boilup flow rate [kmol/min]
D	Distillate flow rate [kmol/min]
S	Side stream flow rate [kmol/min]
R_l	Liquid split ratio
R	Bottom Product flow rate [kmol/min]
$D1$	Prefractionator top product flow rate [kmol/min]
$R1$	Prefractionator bottom product flow rate [kmol/min]
F	Optimal sensitivity
q_F	Liquid feed
p_F	Price of feed [\$/kmol]
p_V	Price of energy [\$/kmol]
p_D	Price of top distillate [\$/kmol]
p_S	Price of side product [\$/kmol]
p_B	Price of bottom product [\$/kmol]
p_R	Price of bottom product [\$/kmol]
c	Candidate controlled variables

Abbreviations

DWC	Divided wall column
DOF	Degrees of freedom
SOC	Self- optimizing control
CVs	Controlled variables
CV1	Primary controlled variables
CV2	Secondary controlled variables
MVs	Manipulated variables
TPM	Throughput manipulator
MPC	Model predictive control
CPU	Central processing unit

CHAPTER 1

Introduction

1.1 Motivation and Literature Review

Distillation is a technic of separating liquid mixtures based on difference in relative volatilities of different components in the mixture. It is one of the most preferred methods of separation in the process industry like petroleum and gas refineries, chemical and petrochemical units. Distillation alone accounts for the major portion of energy consumptions in chemical industries. Meeting the growing energy demand and reducing green-house gas emissions to meet the environmental compliances seek more efficient design and operation of the distillation columns. However, the design improvement to bring down the capital cost should not be overlooked as it can also contribute to significant amount of cost reduction. Therefore, dividing wall columns have gained increasing applications due to their lower energy consumption and investment costs. A dividing wall column (DWC) has a vertical partition that divides the column shell into a pre-fractionator and side draw section. The ternary product dividing wall column is typically called Petlyuk column and the four product dividing wall column is called Kaibel column.

The capital saving in dividing wall column is because of reduced numbers of equipment (one column shell, one reboiler and one condenser) and piping. In addition the reduced equipment and piping also cause significant space saving. Despite the fact that the three product Petlyuk column or dividing wall column can give around 20-30% capitals as well as energy saving (Triantafyllou and Smith 1992, Amminudin, et al. 2001) over conventional distillation column, the commercial application is very limited. The reason for limited use on industrial level is the difficulty in both the operation and control of the divided wall column. The divided wall columns have more steady state degrees of freedom than the conventional column and therefore more difficult to both design and

control. The difficulty in control is also increased because of the increased interactions between the increased numbers of control loops compared to conventional distillation column. Like conventional distillation column, divided wall (Petlyuk) column model is also highly non-linear in nature.

The concept of dividing wall column was introduced by (Wright 1949) as a design alternative to conventional distillation for separating ternary feed. The idea was to use a physical wall separating the feed from side draw section in a single column shell. This could significantly reduce both the capital cost and energy consumption (Wolff and Skogestad 1995). Later, the concept of dividing wall column was first introduced in 1965 (Petlyuk, Platonoy and Slavinskii 1965). Unlike Wright, they did not use a wall; instead they used two-column implementation to prevent remixing effects at the feed location. The reduction in remixing effect caused less thermodynamics loss.

Further other investigators ((Wolff and Skogestad 1995); (Mutalib, et al. March 1998); (Niggemann and Hiller 2010); have conducted rigorous experimental and simulation studies to conduct dynamic studies related to startup as well as normal operation of such systems. Halvorsen and Skogestad introduced the idea of the V_{min} diagram for analyzing the energy consumption for separation the feed components in distillation column (Halvorsen and Skogestad 2003). It is a graphical tool (V_{min} diagrams) which can be used to check the minimum energy requirement for sharp and non-sharp separations in both the conventional and thermally coupled columns. V_{min} diagrams can be created for any mixture assuming a column with a large number of theoretical stages and it is based upon the Underwood equations.

The modes of operation based on operational objective and constraints have been studied by several investigators (Halvorsen and Skogestad 1999, Starndberg June 2011, Ghadrnan, Halvorsen and Skogestad 2011). Strandberg (Starndberg June 2011) considered four different cases of optimal operation of the Kaibel column with feed rate as a degree of freedom. Ghadrnan et al. (Ghadrnan, Halvorsen and Skogestad 2011) extended the investigation of two cases, namely minimizing energy usage for fixed product specifications (Mode-I_{ABC}) and maximizing product purities for fixed boilup (Mode-II₀). Dwivedi et al. (Dwivedi, Halvorsen and Skogestad 2012) mainly focused on the control structure selection for fixed product specifications with minimum energy

usage (Mode-I_{ABC}). Halvorsen and Skogestad (Halvorsen and Skogestad 1999) studied steady-state optimal operation for minimum energy usage (Mode-I_{ABC}) and concluded that energy saving is difficult without a good control strategy. They also discussed candidate feedback variable for self-optimizing control scheme for minimizing the energy usage.

Further, Khanam et al. (Khanam, Shamsuzzoha and Skogestad 2013) have studied the optimal operation of divided wall (Petlyuk) column for fixed energy and non-optimal vapor split ratio R_v (Mode-II₀). The objective cost function in their study was to minimize the sum of impurities and their results showed that for fixed energy and non-optimal R_v , the optimal operation would tend to direct product impurities to the side stream with both fixed and variable R_v .

1.1 Scope of Thesis Work

In this work, the study on the three-product divided wall column has further been extended to the control structure design of the column. The main work is focused on selecting the primary controlled variables by implementing self-optimizing control on the column. The selection of appropriate controlled variables is very important task in self-optimizing control. Also, the selected controlled variables c can be individual measurement or the linear combination of measurement y , i.e. $c = Hy$. c is kept at constant set-point by using feedback control which would cause loss due to disturbances and also loss due to implementation error.

The pseudo/steady state loss evaluation using different methods as cited in recent literature by Yelchuru and Skogestad (Yelchuru and Skogestad 2012), (Yelchuru 2012) and in other previous work { (Halvorsen, Skogestad and Morud, et al. 2003), (Alstad, Skogestad and Hori 2009), (Alstad 2005) and (Cao and Kariwala 2008)} can be tested to evaluate loss caused by self-optimizing control. Mainly, the loss can be evaluated using different measurement combinations H based on the average loss criterion and exact local method. However, the selection of variables can also be validated by using non-linear model for large disturbances.

In addition, plantwide control procedure can be applied to evaluate different modes of operations based on active constraints.

1.2 Thesis Overview

- **CHAPTER 2** : The fundamentals of distillation used in this study have been presented and also various arrangement of three-product separation (with schematic diagrams) has been illustrated.
- **CHAPTER 3** : The theory of Skogestad's plantwide control procedure used in this study has been presented. Also the theory of self-optimizing control, selection of controlled variables for unconstrained degrees of freedom and methods to evaluate loss at pseudo/steady-state has been described. The method of tuning the controller for dynamic simulation has also been briefly discussed. Further, the sequential tuning method for tuning multivariable system has been briefly written down.
- **CHAPTER 4** : In this chapter, the process has been described and plant process data for case study has been given. This chapter also explains how the plantwide control procedure for control structure design and self-optimizing control has been implemented on the three-product divided wall column.
- **CHAPTER 5** : In this chapter the simulation procedure to retrieve results obtained in this work has been given.
- **CHAPTER 6** : This chapter comprises of the results and discussion from this work.
- **CHAPTER 7** : This chapter concludes the work with suggestions on possible further work.

1.3 Publications

1. Ambari Khanam, M. Shamsuzzoha, Sigurd Skogestad, “Control structure design of divided wall column for optimal operation”, 10th International Conference for DISTILLATION & ABSORPTION 14-17 September 2014, Friedrichshafen, Germany.(accepted for final submission)
2. Ambari Khanam, M. Shamsuzzoha, Skogestad, Sigurd Skogestad, “Optimal operation and control of divided wall column”, 24th European Symposium on Computer Aided Process Engineering— ESCAPE 24 June 15-18, 2014, Budapest, Hungary. (accepted for final submission)
3. Ambari Khanam, M. Shamsuzzoha, Skogestad, S, “Operation of energy efficient divided wall column”,23rd European Symposium on Computer Aided Process Engineering – ESCAPE 23 June 9-12, 2013, Lappeenranta, Finland.
4. Ambari Khanam, M. Shamsuzzoha, Skogestad, S, “Design and operation of energy efficient divided wall column”, 9th European Congress of Chemical Engineering –21-24 April, 2013, The Hague, The Netherlands.

CHAPTER 2

Distillation Fundamentals

In this chapter, the distillation theory used in this study has been briefly discussed and also various column sequences to achieve the three-product separation or certain separation have been illustrated.

2.1 Distillation

Distillation is the process of separating liquid mixtures into various components based on the difference in their boiling point. Separation becomes easier with increase in relative volatilities between the components. However for the given components, separation can still be increased by increasing the number of stages in the column or by increasing the energy (reflux) relative to the feed flow rate (S. Skogestad 1997) .

2.1.1 Relative Volatility

The thermodynamic definition for relative volatility in a single stage is the ratio of pure component vapor pressure and the ratio of the activity coefficient in the liquid phase as given by **Eq.(2.1)** (Robbins 2011).

$$\alpha = \frac{\gamma_1 p_1}{\gamma_2 p_2} = \left(\frac{y_1}{y_2} \right) / \left(\frac{x_1}{x_2} \right) \quad (2.1)$$

where:

α = relative volatility

γ = activity coefficient in the liquid phase

p = pure component vapor pressure

x = mole fraction in liquid phase

y = mole fraction in vapor phase

1 & 2 are subscripts for component 1 and component 2 respectively

2.1.2 Separation Factor

The separation factor S in a distillation column is the ratio of light key to heavy key component in the distillate divided by the ratio of light key to heavy key components in the bottoms as given by **Eq. (2.2)**:

$$S = \left(\frac{x_L}{x_H} \right)_T / \left(\frac{x_L}{x_H} \right)_B \quad (2.2)$$

Where, x is the mole fraction of light component L and heavy component H respectively in the top T and bottom B of the column (S. Skogestad 1997) and (Robbins 2011).

2.1.3 Assumptions

The model for this study is based on the following assumptions:

- The feed is an ideal mixture
- Equilibrium on all stages
- Constant relative volatility
- Negligible vapor holdups
- One feed and three products
- Constant internal molar flows
- Total condenser

2.1.3.1 Constant Relative Volatilities

The relative volatility between components i and j is given by **Eq. (2.3)** (Halvorsen 2001):

$$\alpha_{i,j} = \frac{\left(\frac{y_i}{x_i}\right)}{\left(\frac{y_j}{x_j}\right)} = \frac{K_i}{K_j} \quad (2.3)$$

The K values for components i and j are equilibrium constants which depend on both pressure and temperature. The temperature in the column varies from top to bottom, highest in the bottom and lowest in the top. For feed which is an ideal mixture containing three components i , j , and k , the following assumption can be made for the calculation of relative volatilities (In this work A (lightest), B (medium) and C (heaviest) (Halvorsen 2001):

- The relative volatility between any two components is the geometric average of the relative volatility at the highest temperature and lowest temperature at both ends of the column.
- The relative volatilities of three components i , j and k are calculated with respect to the heaviest component (least volatile).

2.1.3.2 Equilibrium on Stages

Equilibrium on all stages means the vapor composition y and the liquid composition x are considered to be in equilibrium on all theoretical stages.

In a two phase (liquid and vapor) system with n components the mole fraction x in liquid phase and the mole fraction y in vapor phase:

$$\sum_{i=1}^n x_i = 1 \quad \text{and} \quad \sum_{i=1}^n y_i = 1$$

The VLE (vapor liquid equilibrium) relationship in terms of relative volatility (using the heaviest component as the reference point), liquid mole fraction and vapor mole fraction is given by **Eq. (2.4)**:

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

Considering a two component system with x as the light component, the above equation can be rewritten as **Eq. (2.5)**

$$y = \frac{\alpha x}{1 + (1 - \alpha)x} \quad (2.5)$$

2.1.3.3 Constant Molar Flows:

Constant molar flow means that both liquid flow rate and vapor flow rate on each stage of the column are same except at the stage where feed is added or the product is withdrawn. The liquid and vapor flow rate on consecutive stages are given by **Eq. (2.6)** below:

$$L_n = L_{n+1} = L \quad \& \quad V_{n-1} = V_n = V \quad (2.6)$$

The above assumptions are valid for the separation of only similar components because in that case heats of vaporization are similar and no energy balance is required (Alstad 2005).

2.1.3.4 Estimation of Temperature from Composition and Boiling points

The temperature on each tray is approximated by the linear weightage of the boiling temperatures of three components with their mole fraction:

$$T = \sum_i^3 x_i T_i \quad (2.7)$$

2.1.3.5 Linearized Liquid Flow Dynamics

The liquid flow dynamics are modeled as given below, **Eq. (2.8)**

$$L_i = L_{0,i} + \frac{M_i - M_{0,i}}{\tau_L} + (V_{i-1} - V_{0,i-1})\lambda \quad (2.8)$$

M_i and $M_{0,i}$ are holdup on stage i and nominal holdup on stage i respectively, (S. Skogestad 1997)

2.2 The column in Sequence

Many complex column arrangements can be used in order to achieve a separation of multicomponent mixture. It mainly depends on a whole host of variables including the pressure and temperature under which the separation takes place. Once all considerations have been taken into account, certain trade-offs need to be made in order to achieve an optimum design. The most important factors that affect the design of the separation process are operability, controllability and flexibility. Some of the different column sequences to achieve a certain separation are described below:

For separating a three or more component feed using conventional distillation column, the two most commonly used arrangements are the direct and the indirect sequence.

2.2.1 Direct Sequence

The sequence represented in **Figure 2-1** is used when the feed has a high concentration of the lightest components or when the separation of the middle

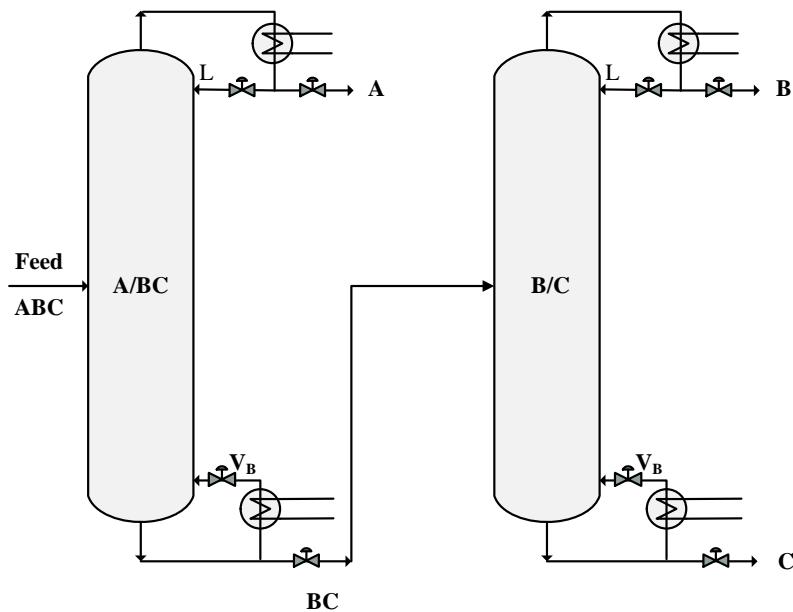


Figure 2-1: Direct column sequence for the separation of three products

distillate and the heavy product is slightly more difficult than that of the light and middle distillate. The light component is taken off as a distillate and the rest of the product is sent to a second column to undertake the subsequent separation. The columns are separated by a single liquid stream so they may be operated at different pressures in order to perform the optimum separation.

2.2.2 Indirect Column Sequence

Indirect arrangement as shown in **Figure 2-2** is most often used when the feed has a high concentration of the heavy product or when the separation of the light from the middle distillate is relatively more cumbersome. The heavy product is first separated out then the distillate is fed to a second column for further separation. For the vapor from a partial condenser the pressure in the second column needs to be lower than that of the first column for natural flow of the vapor, else a compressor would be needed between

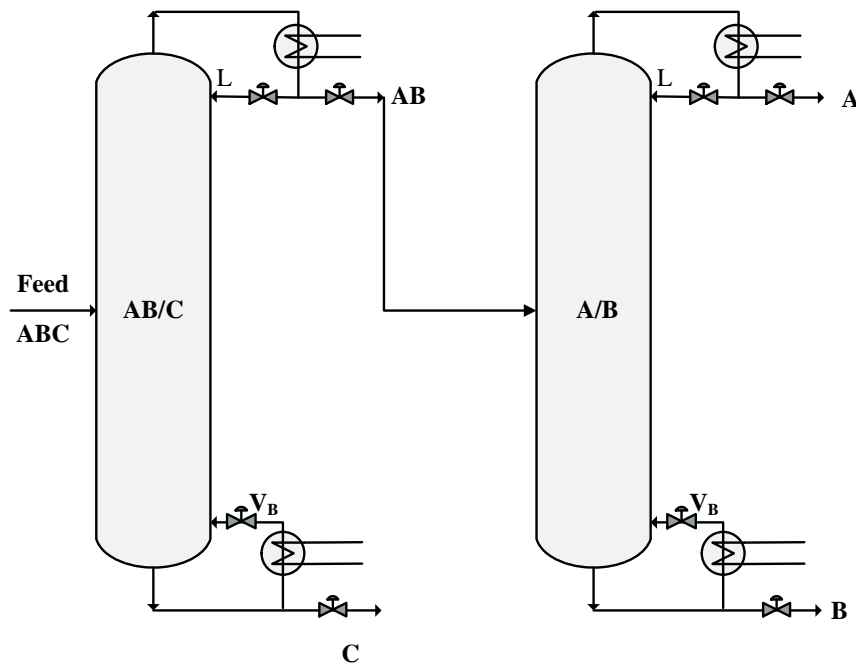


Figure 2-2: Indirect column sequence for the separation of three products

the columns. If a total condenser were used then the pressures in each column can be treated and optimized independently. The total number of columns required for a separation of a mixture using direct or indirect sequence is $N-1$, where N is number of components in the feed mixture.

Distributed Column Sequence : This is capital intensive arrangement and requires three distillation columns for the separation. It is considered most often when the required light, heavy and middle products are all close boiling materials and the separation can be done at low temperatures using lower quality utilities. This arrangement would also be considered when there is a high concentration of middle distillates in the feed. This configuration separates out the entire light component in the tops of the first column and the entire heavy product in the bottoms with the middle distillates being split between both these streams. The two subsequent columns separate light from middle and middle from heavy products.

Side Rectifier: A rectifier is thermally linked to the main column. This coupled column uses one reboiler to generate the vapor for both the columns but two condensers for liquid rectification. The entire system has to operate at the same pressure, but the pressure in the main column is slightly higher than that in the rectifier to accommodate for the natural flow of vapor. A system similar to the Side Rectifier would be the Side Stripper. The difference being that in this arrangement there are two reboilers and only one condenser. In this case the stripping section operates at a slightly higher pressure for natural vapor flow to occur.

Pre-fractionator: This configuration splits the feed into two feeds for the second column that has a side-draw as well. There are some similarities between this arrangement and the distributed sequence. This configuration can be thought of a coupling of the distributed arrangement and the removal of a condenser and a reboiler. This strategy is preferred when there is a large amount of middle distillate in the feed or if the splits between all fractions in the feed are difficult. Both columns may operate at different

pressures in order to take advantage of utilities available at different temperatures for the Pre-fractionator and main column sections.

2.2.3 Thermodynamic Implementation of Three-Product Petlyuk Column

The Petlyuk configuration represents an arrangement that can separate three or more components using a single reboiler and a single condenser. This configuration has even more thermal coupling than the pre-fractionator which increases efficiency; this also means that there are greater internal flows with no hold-ups due to not having an intermediate reboiler or condenser in the Petlyuk column. The exchange of vapor and liquid between the columns poses strict pressure and operability constraint **Figure 2-3**,

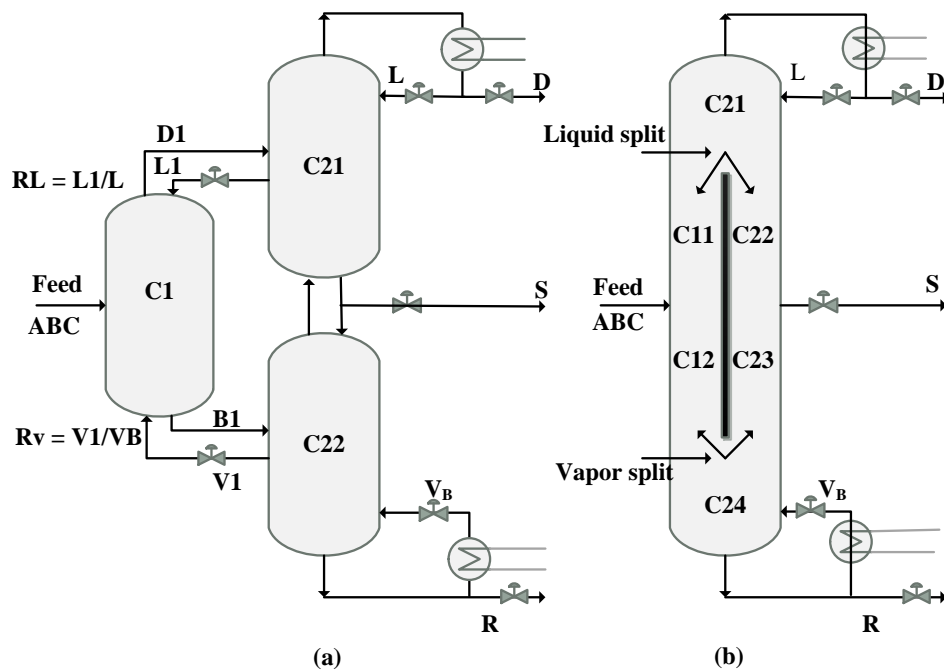


Figure 2-3: (a) Thermodynamically equivalent implementations of three-product DWC (b) DWC implementation

represents the thermodynamically equivalent implementation of three products divided wall column configuration. It is the most compact distillation column for the separation of these products that allows for both considerable energy and capital saving. There is a partition between the feed and side-draw sections of the column, which provides greater capacity and increased separation efficiency yet still a normal side-draw column. This column is thermodynamically identical to the Petlyuk column provided that there is negligible heat transfer across the dividing wall section of the column.

CHAPTER 3

Optimal Selection of Controlled Variables

Plantwide control deals with the most basic questions about the decision making related to optimal operation and control –“which variables should be controlled, which variables should be measured, which inputs should be manipulated and which link should be made between them” (Foss 1973). This Chapter briefly describes the plantwide control procedure (Larsson and Skogestad 2000), (S. Skogestad 2000), (S. Skogestad 2004), (Halvorsen, Skogestad and Morud, et al. 2003). Most importantly, the theory related to the selection of controlled variables which is the essence of this work has been discussed. To validate the selection of candidate controlled variable the method to evaluate loss using self-optimizing control scheme has been explained (Yelchuru and Skogestad 2012) (Alstad and Skogestad 2007), (Alstad , Skogestad and Hori 2009) and (Halvorsen, Skogestad and Morud, et al. 2003).

3.1 Plantwide Control Procedure

There are various literatures on the plantwide control procedure. Skogestad’s economic plantwide control structure design procedure has been applied in this study and is discussed here, (S. Skogestad 2013). A typical control system hierarchy divided into several layers based on the time scale is given in **Figure 3-1**. Each layer has its own goal and typically each lower layer maintains the setpoints decided by the layer above. The procedure typically does not guide for control loop behavior and tuning rather it emphasizes on the important structural decisions as given below:

- *Selection of controlled variables (“outputs”)*

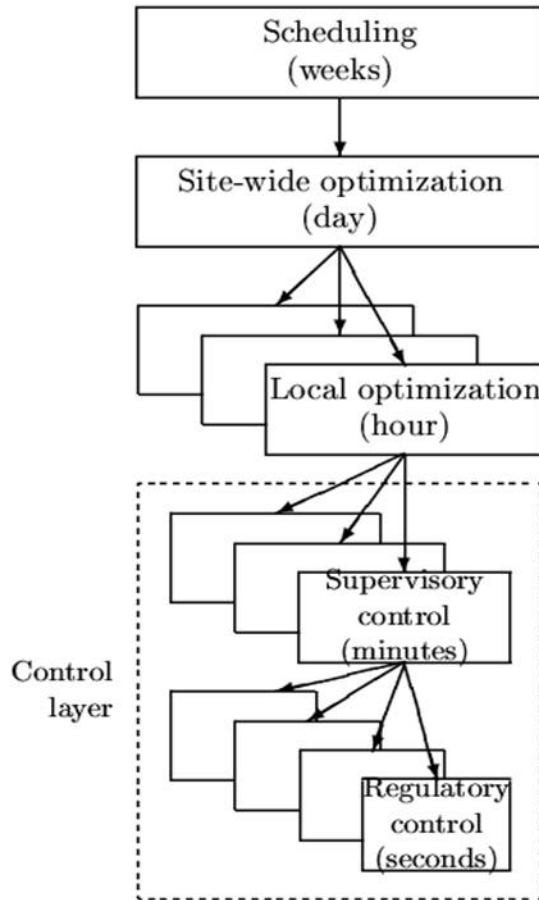


Figure 3-1: Typical control hierarchy in a chemical plant (Larsson and Skogestad)

- *Selection of manipulated variables (“inputs”)*
- *Selection of (extra) measurements*
- *Selection of control configuration* (structure of overall controller that interconnects the controlled, manipulated and measured variables)
- *Selection of controller type* (LQG, H-infinity, PID, decoupler, MPC etc.).

The above structural decisions useful in designing the control structure are also cited in various studies (Foss 1973), (Morari 1982), (S. Skogestad 2000), (S. Skogestad 2004) and (Skogestad, and Postlethwaite 1996).

Skogestad proposed two approaches for economic plantwide procedure for control structure design analysis (S. Skogestad 2013). Only those steps have been elaborated here that have been used in this work:

3.1.1 Top- Down Analysis (Economics)

The top-down analysis suggests step by step approach for plantwide control structure design. There are four steps and are briefly explained below:

Step 1: Define Optimal Operation

The first step of Skogestad top-down analysis is to define the operational objective subjected to operational constraints (S. Skogestad 2000) . The typical operational objective is the plant's economics subjected to minimizing the cost or maximizing the profit at steady-state. The typical cost function in chemical plants is given below:

$$J = \text{Cost feed} + \text{cost energy} - \text{value products} \quad (3.1)$$

The mathematical representation of the steady-state optimal operation subjected to constraints is given below by **Eq. (3.2)**

$$\min_{u_s} J(x, u_s, d) \quad (3.2)$$

The constraints are given by **Eq. (3.3)** and **Eq. (3.4)**.

$$g_1(x, u_s, d) = 0 \quad (3.3)$$

Where **Eq. (3.3)** denote the model equations,

$$g_2(x, u_s, d) \leq 0 \quad (3.4)$$

Eq. (3.4) denotes operational constraints. In the above equations, $x \in R^{n_x}$ are state variables, $u_s \in R^{n_{u_s}}$ denote the steady-state degrees of freedom. $d \in R^{n_d}$ are disturbances that are inevitable and cannot be manipulated or controlled. The available degrees of freedom u^T , comprises of both steady-state degrees of freedom and degrees of

freedom which do not have any effect on steady-state operation. For example in a distillation column the degrees of freedom which are used to control the levels in condenser and reboiler tank do not have any effect on steady-state operation.

Step 2: Optimization (offline-calculations)

The second step of top-down analysis is the optimization using offline calculations. The task in this step is subdivided into two steps:

Step 2a: Degrees of Freedom Analysis:

Since the plant economics is evaluated based on steady-state conditions therefore the identification of degrees of freedom is done at steady-state. The steady-state degrees of freedom are important in analyzing the number of primary controlled variables (define primary CVS, for economics). There are three methods which are commonly used to obtain steady-state degrees of freedom (N_{SS}):

1. Equation-counting: In this method N_{SS} is the difference of number of variables and number of equations or specifications.
2. Valves-counting:

$$N_{SS} = N_{valves} - N_{0_{SS}} - N_{specs}$$

where N_{valves} is the dynamic degrees of freedom, $N_{0_{SS}}$ is the number of variables with no steady-state effect and N_{specs} is the number of equality specifications.

3. Potential numbers for some units like heat exchangers, condensers, columns, vessels etc.

Amongst above three methods, valves-counting and potential number for some units are simpler and easier to use.

Step 2b: Optimize for Expected Disturbances

In this step, the operation is optimized with respects to degrees of freedom u , for expected disturbances d and the region of active constraints are found. The main idea behind this is to prepare in advance how one should deal with expected disturbances including the change in prices of products, energy and feed.

Step 3: Implementation of Optimal Operation

In this step, the task is to select primary controlled variables (CV1s) in order to implement the optimal operation. The numbers of primary CVs is same as the available steady-state degrees of freedom. It is found that at the optimum some of the constraints are active and therefore they should be controlled first. The reason behind it is that controlling active constraints in first place cause linear loss. The constraints which are not active should be scrutinized as they give quadratic loss (Halvorsen, Skogestad and Morud, et al. 2003).

In this step after controlling the active constraints, the remaining unconstrained degrees of freedom are used for self-optimizing control. By implementing self-optimizing control, real time optimization is not needed to calculate new setpoints c_s in case of new disturbances. Instead, self-optimizing control emphasizes on the selection of CV1 to be kept constant by manipulating u in a feedback fashion, as shown in **Figure 3-2**. In

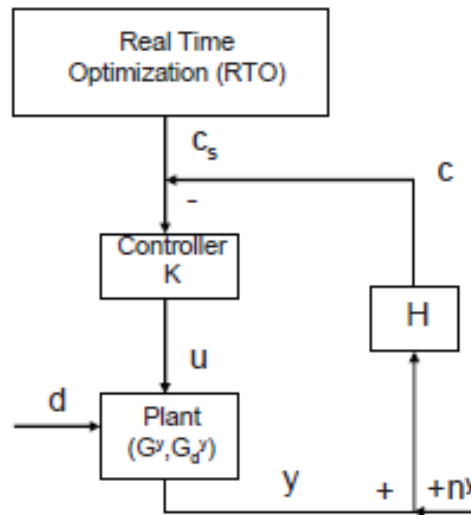


Figure 3-2: Feedback implementation of optimal operation with separate layers for optimization and control, (Kassidas, Patry and Marlin 2000) and (Engell 2007)

case of any disturbance (d), the controller K tries to maintain the controlled variables c at their setpoint c_s .

Step 4: Where to Set the Production Rate (TPM)

This is the last step of Skogestad (S. Skogestad 2013) top-down analysis of the plant wide control structure design procedure. This is the link between top-down analysis (for economics) and the bottom-up analysis (for stabilization). The “TPM” term means throughput manipulator and is generally meant to be the “gas pedal” of the process. TPM is generally some flow rate however it is not necessary always like in a reactor case TPM might be some temperature. Generally there is one TPM in a plant but there can be more than one in case of multiple feed and parallel units.

3.1.2 Bottom-Up Analysis (Stabilization)

Step 5: Regulatory Control Layer

The regulatory control layer is needed for stabilization of the plant against future disturbances. In this layer pairing is made between the secondary controlled variables (CV2) and manipulated variables for the stable operation of the plant.

Step 6: Supervisory Control Layer

The secondary controlled variables (CV2) of the regulatory control layer act as inputs to the supervisory control layer. The main purpose of this layer is to maintain the primary controlled variables c at their setpoint c_s subjected to optimal operation.

Step 7: Real Time Optimization

The real time optimization is used (time scale is hour) to re-optimize operation and find new optimal points caused by change in disturbances from the optimum.

3.2 Self-optimizing Control

“Self-optimizing control is when we achieve acceptable loss (in comparison with truly optimal operation) with constant setpoint values for the controlled variables (without the need to re-optimize when disturbances occur” (S. Skogestad).

In the above definition of self-optimizing control, the acceptable operation means the loss by keeping the constant setpoints policy as given by **Eq. (3.5)**:

$$Loss = J_u(u, d) - J_{opt}(u_{opt}(d^*), d^*) \quad (3.5)$$

$J_u(u, d)$ is the cost when the controlled variables are kept at constant setpoints and $J_{opt}(u_{opt}(d^*), d^*)$ is the optimal cost. **Figure 3-3** illustrates the cost function J as a function of input u (unconstrained degrees of freedom) and disturbance d . $u_{opt}(d)$ and $u_{opt}(d^*)$ are the optimal inputs for disturbance d and d^* . The figure also shows the loss by keeping input u constant at $u = u_{opt}(d^*)$ in case of disturbance d . In self-optimizing control, the input u is updated to keep the measurement or combination of measurements Hy_m at setpoint c_s by a feedback diagram as shown in **Figure 3-4**.

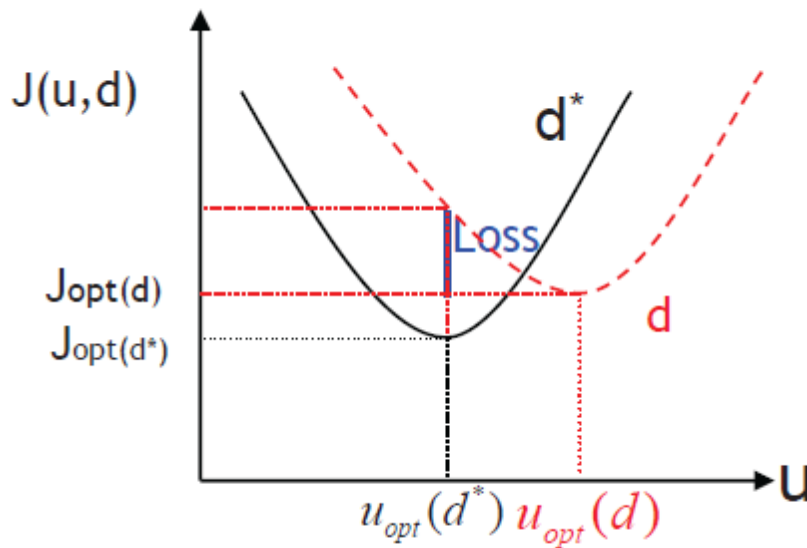


Figure 3-3: Cost function as a function of disturbance d & d^* and inputs u , (Yelchuru 2012)

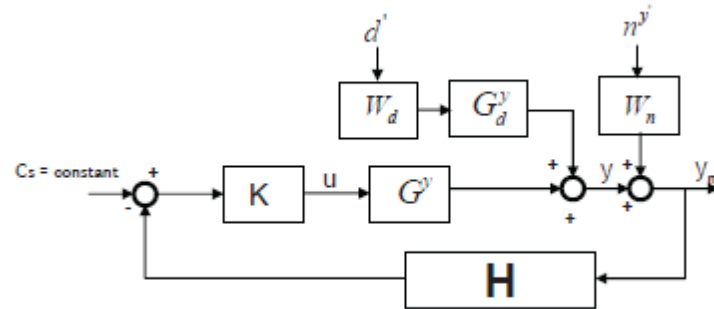


Figure 3-4: The feed-back control diagram for self-optimizing control, (Yelchuru 2012)

In self-optimizing control a good candidate controlled variables c should have following properties, (S. Skogestad) :

- The optimal value of c should be insensitive to disturbances
- c should be easy to measure and control (i.e. its implementation error should be small)
- The value of c should be sensitive to changes in the degree of freedom (i.e. steady-state gain from u to c should be large).

3.2.1 Methods for Loss Evaluation

In this study local methods have been used for identifying the promising primary controlled variables and further they have been also tested on the non-linear model. Local methods are based on the local analysis of loss and linearized steady-state model around optimal operating points. These methods are based on the assumptions that the plant's economics are governed by the pseudo/steady-state behavior, (Yelchuru 2012).

As explained above the self-optimizing control proposes the concept of minimizing the loss by keeping certain setpoints constant. The simplified loss expression can be written as $\{L = J - J_{opt}(d)\}$. Here, the idea is to minimize the loss caused by self-optimizing

control unlike minimizing cost J . The loss minimization using local methods are termed as minimum loss method by Skogestad and Yelchuru, (Yelchuru and Skogestad 2012).

3.2.1.1 Variable and Notations

- $u \in R^{n_u}$: unconstrained steady-state degrees of freedom also called inputs
- $d \in R^{n_d}$: disturbances
- $y \in R^{n_y}$: all available measurements, including inputs and measured disturbances
- n^y : measurement errors (noise), $y_m = y + n^y$.
- $c \in R^{n_c}$: $n_c = n_u -$ selected controlled variables , $c = Hy$

3.2.1.2 Cost Function

The unconstrained cost function is written below (Yelchuru and Skogestad 2012):

$$J(u, d) = J(u^*, d^*) + [J_u^* \quad J_d^*] \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix} + \frac{1}{2} \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix}^T \begin{bmatrix} J_{uu}^* & J_{ud}^* \\ J_{ud}^T & J_{dd}^* \end{bmatrix} \begin{bmatrix} \Delta u \\ \Delta d \end{bmatrix} + \quad (3.6)$$

- $\Delta u = u - u^*$ and $\Delta d = d - d^*$ are expressions for deviation from nominal optimal point u^* & d^*
- J_u^* and J_d^* are first derivative of cost with respect to u and d respectively.
- J_{uu}^* , J_{ud}^* and J_{dd}^* are second derivative of cost with respect to u, u and d and d respectively at u^* and d^* .

Since, the nominal point is assumed to be giving the minimum optimal cost therefore, $J_u^* = 0$. Further, to simplify the problem, it is also assumed that the nominal inputs and disturbances $(u^*, d^*) = (0,0)$ and hence $(y^* = 0)$. By applying these assumptions to the cost function as given by **Eq. (3.6)**, it is found that the values of J_d^* and J_{dd}^* are not required for finding the optimal measurement combination matrix H .

3.2.1.3 Assumptions

The finding of optimal H and loss evaluation is based on the following assumptions:

- u spans the unconstrained subspace and does not consists of the constrained degrees of freedom used to control active constraints .
- The required number of controlled variables is same as the number of unconstrained degrees of freedom ($n_c = n_u$). This ensures that HG^y is a square matrix ($n_u \times n_u$).
- In order to get off-set free control of all primary controlled variables, the number of independent measurements should be greater than the number of unconstrained degrees of freedom i.e. ($n_y \geq n_u = n_c$).
- $d = W_d d'$, where W_d the diagonal matrix is such that the diagonal elements are the expected magnitude of each disturbances and the magnitude of d' is one.
- $n^y = W_{n^y} n^{y'}$, where W_{n^y} is the diagonal matrix such that the diagonal elements are the magnitude of the measurement noise and the magnitude of vector $n^{y'}$ is one.

3.2.2 Re-defining the Minimum Loss method

The optimal matrix H is obtained by keeping measured controlled variables c at constant setpoint c_s by adjusting u using feedback control as shown in **Figure 3-4**.

$$c_m = H(y + n^y) = c_s = 0 \quad (3.7)$$

H matrix is calculated such that it minimizes the loss as given below by **Eq. (3.8)**:

$$L = J(u, d) - J_{opt}(d) \quad (3.8)$$

The loss is minimized for the expected disturbance d and the measurement noise n^y . The unit magnitude of disturbance and the measurement noise is defined below for two different cases of loss:

1. Worst -case loss, L_{wc} : In this case the combined normalization vectors for disturbances and measurement noise have 2-norm less than 1, **Eq. (3.9)**:

$$\left\| \begin{bmatrix} d' \\ n^{y'} \end{bmatrix} \right\|_2 \leq 1 \quad (3.9)$$

2. Average loss, $L_{avg} = E(L)$: In this case, normal distributed set is given below:

$$\begin{bmatrix} d' \\ n^{y'} \end{bmatrix} \in \mathcal{N}(0,1) \quad (3.10)$$

$E(\cdot)$ is expectation operator.

3.2.2.1 Solution to Minimum Loss Problem (Exact Local Method)

The solution to minimum loss problem comprises of expression for optimal input, u_{opt} , expression for loss L in terms of $u - u_{opt}d$ and optimal sensitivities F ($F1$ in this study), (Halvorsen, Skogestad and Morud, et al. 2003).

Optimal input (u_{opt}): The expansion of gradient J_u around optimal point, $(u^*, d^*) = (0,0)$ gives the optimal input as a function of disturbance d , **Eq. (3.11)** :

$$u_{opt} = -J_{uu}^{*-1} J_{ud}^* d \quad (3.11)$$

The expression for loss is given by the following equation, **Eq. (3.12)**:

$$L(u, d) = J(u, d) - J_{opt}(d) = \frac{1}{2} z^T z = \frac{1}{2} \|z\|_2^2 \quad (3.12)$$

where,

$$z \triangleq J_{uu}^{1/2} (u - u_{opt}(d)) \quad (3.13)$$

Optimal sensitivity, (F): The expression for optimal sensitivity of the outputs (measurements) with respect to disturbances is given by F below:

$$F = (-G^y J_{uu}^{-1} J_{ud} + G_d^y) \quad (3.14)$$

Also, F can be directly calculated from its definition, **Eq.(3.15)** :

$$F = \frac{dy_{opt}}{dd} \quad (3.15)$$

The expression of loss as a function of disturbance and noise is given by the following equations:

$$L = \frac{1}{2} z^T z \quad (3.16)$$

where ,

$$z = \underbrace{J_{uu}^{1/2} (HG^y)^{-1} HY}_{M(H)} \begin{bmatrix} d' \\ n^{y'} \end{bmatrix} \quad (3.17)$$

And the expression Y in the above equation is the optimal variation in the candidate controlled variables or measurements due to disturbances and measurement noise:

$$Y = [FW_d \ W_{n^y}] \quad (3.18)$$

W_d and W_{n^y} are the diagonal matrices representing the magnitude of disturbances and measurement noise.

Worst-case and average loss for a given H:

The worst-case loss (Halvorsen, Skogestad and Morud, et al. 2003) is given by the following equation:

$$L_{wc} = \frac{1}{2} \bar{\sigma}(M)^2 \quad (3.19)$$

and the average loss is given by, (Kariwala, Cao and Janardhanan 2008):

$$L_{avg} = E(L) = \frac{1}{2} \|M\|_F^2 \quad (3.20)$$

where

$$M(H) = J_{uu}^{1/2} (HG^y)^{-1} HY \quad (3.21)$$

$\bar{\sigma}(M)$ denotes the maximum singular value (induced 2-norm) of the matrix $M(H)$ and $\|M\|_F = \sqrt{\sum_{i,j} M_{i,j}^2}$ is the frobenius norm of the matrix M . The use of norm to analyze loss is known as “*The exact local method*” (Halvorsen, Skogestad and Morud, et al. 2003). These loss expressions are for given H .

(Kariwala, Cao and Janardhanan 2008) have proved that the H that minimizes average loss as given in **Eq.(3.20)** is super optimal because the same H also minimizes the worst case loss in **Eq. (3.30)**. Hence, in this work only the minimization of frobenius norm is considered, (Yelchuru 2012).

There are several different methods to evaluate loss at steady-state however in this study three different methods have been used to evaluate loss at the steady-state. Of all these three methods the exact local method has been explained above and the remaining two methods are explained below:

3.2.2.2 The Maximum Minimum Singular Rule

In this work, the maximum minimum singular value rule of Halvorsen et al. (Halvorsen, Skogestad and Morud, et al. 2003) and (Skogestad, and Postlethwaite 1996) has been used to select the best set of measurements (stage temperatures) giving the minimum loss. The selection is based on scaled steady-state gain from inputs to the candidate controlled variables. The steps to calculate scaled gain matrix are as follows:

- The model is linearized around optimal point in order to get measurement dependent on u and d and is given by the following equation, **Eq. (3.22)** :

$$y = G^y u + G_d^y d = \tilde{G}^y \begin{bmatrix} u \\ d \end{bmatrix} \quad (3.22)$$

G^y and G_d^y are the transfer functions but for calculating H only the steady-state gains have been used, (Yelchuru 2012).

- Using the linear model the input u_j is scaled i.e. $u_{scl,j} = 1/\sqrt{[J_{uu}]_{jj}}$.
- The optimal variation ($\Delta y_{opt,i}$) due to disturbances is calculated for each candidate controlled variable i.e.

$$\Delta y_{opt,i} = [G^y J_{uu}^{-1} J_{ud} - G_d^y]_i d$$

- The expected measurement noise n_i is obtained for each candidate controlled variables
- The scaled candidate controlled variable is the sum of the magnitudes of optimal variation and measurement noise, i.e. $c_{scl,i} = |\Delta y_{opt,i}| + |n_i|$.
- The scaling matrix is then computed, $D_c = diag\{c_{sc,i}\}$ and $D_u = diag\{u_{scl,j}\}$ and finally the scaled gain is obtained i.e. $G' = D_c^{-1} G D_u$.

The value of scaled gain is then used to find the set of temperatures with maximum minimum singular value by using bi-directional branch and bound method by Cao and Kariwala, (Cao and Kariwala 2008). The worst case loss using this method is given by the following expression:

$$L_{wc} = \frac{\alpha}{2} \frac{1}{\underline{\sigma}((G'))^2} \quad (3.23)$$

Here constant $\alpha = \bar{\sigma}(J_{uu})$ is independent of the choice of controlled variable and $\underline{\sigma}(G')$ is the minimum singular value of G' and the maximum singular value $\bar{\sigma}$ is induced 2-norm of a matrix. Thus, to minimize the worst case loss, those controlled variables should be selected which would have maximum minimum singular value. The loss calculated by **Eq. (3.23)** is less accurate than the loss calculated by using **Eq. (3.19)** and **Eq. (3.20)** therefore it is recommended to use the later equations for more accurate values of loss.

3.2.2.3 Null Space Method

The null space method as proposed by Alstad and Skogestad (Alstad and Skogestad 2007) gives measurement matrix H such that $HF = 0$. This method is valid provided numbers of available measurements are more than the sum of unconstrained degrees of freedom and the disturbances ($n_y \geq n_u + n_d$). In such case it is always possible to find a non-trivial H in the left null-space of F resulting in zero loss. In addition it also neglects the effect of measurement noise i.e. $Y = [FW_d \ 0]$. The null space method gives combination of measurement and perfect disturbance rejection.

3.2.3 Loss Evaluation form Dynamic Simulations (Validation)

The loss caused by keeping individual measurement or combinations of measurements as obtained from steady-state self-optimizing control can be validated by dynamic simulation using feedback control. The loss occurring due to disturbances can be the basis for the overall performance of the selected controlled variables.

3.2.3.1 Controller Tuning

For tuning of controllers SIMC tuning rules were used in this work (S. Skogestad 2013). An approximate first order model time-delay model is given below:

$$g_1 = \frac{k}{\tau_1 s + 1} e^{-\theta s} = \frac{k'}{s + \frac{1}{\tau_1}} e^{-\theta s} \quad (3.24)$$

Where

$$k' = \frac{k}{\tau_1} \quad (3.25)$$

- k is the plant gain
- τ_1 is the dominant lag time constant
- θ is the time delay

- s is the Laplace parameter.

There are three methods to obtain the above parameters for controller tuning:

1. Open -loop step response
2. Closed -loop set-point response with P-controller
3. Approximation of effective delay using half rule from detailed model

3.2.3.2 First Order Process

The step response for the first order process model is shown in the **Figure 3-5**. The steady-state gain can be calculated as follows:

$$k = \frac{\Delta y(\infty)}{\Delta u} \quad (3.26)$$

By giving a step change in the manipulated variable or input, all the tuning parameters can be easily obtained. In the given **Figure 3-5**, θ is the time duration on x-axis for which output does not change after step change in input. The time constant τ_1 is the time taken corresponding to 63% of the output value y on y-axis.

The SIMC tuning rule for first order process model is given below in **Eq. (3.27)** and **Eq. (3.28)**

$$k_c = \frac{1}{k} \frac{\tau_1}{\tau_c + \theta} = \frac{1}{k'} \frac{1}{\tau_c + \theta} \quad (3.27)$$

$$\tau_I = \min\{\tau_1, 4(\tau_c + \theta)\} \quad (3.28)$$

In the above equations k_c is the controller gain, τ_I is the integral time and τ_c is closed loop time constant which is used as tuning parameter for tight controller tuning or de-tuning. $\tau_c = \theta$ is a good choice as an initial guess.

3.2.3.3 The Integrating Process

In case, the lag time more than eight times greater than θ , the first order response is then approximated as an integrating process and the tuning parameters are given below:

$$k_c = \frac{1}{k'} \frac{1}{\tau_c + \theta} \quad (3.29)$$

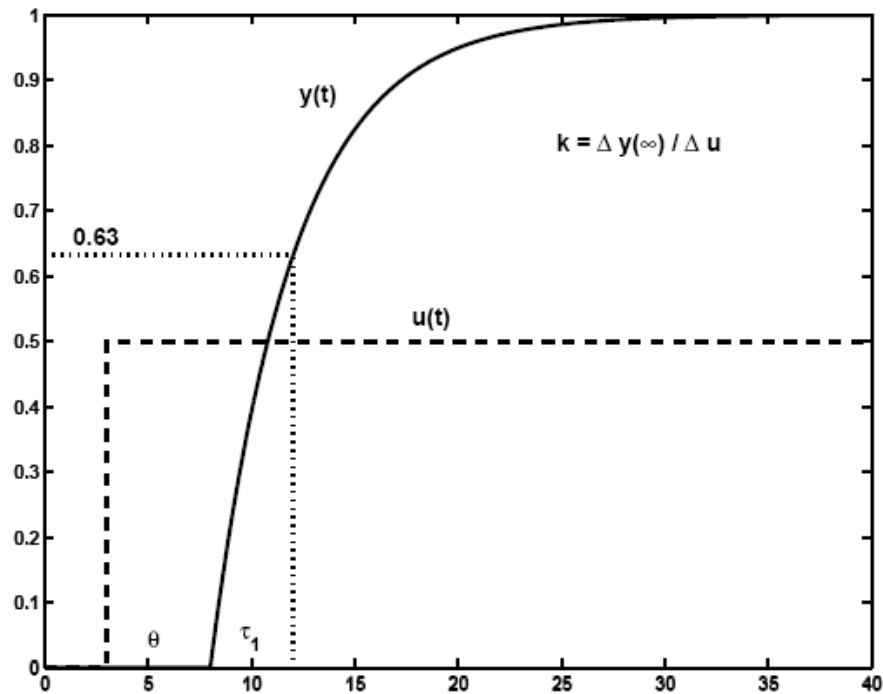


Figure 3-5: Open loop step -response for first order process model (S. Skogestad 2013)

where

$$k_c = \frac{1}{k'} \frac{1}{\tau_c + \theta} \quad (3.30)$$

$$k' = \frac{\Delta y / \Delta t}{\Delta u} \quad (3.31)$$

and

$$\tau_I = 4(\tau_c + \theta) \quad (3.32)$$

3.2.3.4 The sequential Design of Decentralized Control

For the design of a single-input-single-output controller for each loop in a multivariable system, Hovd and Skogestad, (Hovd and Skogestad 1994) have suggested closing and tuning one loop at a time both for online tuning as well as using the process model.

CHAPTER 4

Control Strategies for Divided Wall Column

This chapter describes the system under study and also illustrates the implementation of economic plantwide control procedure and self-optimizing control on the system. The system here refers to the three-product divided wall column .

4.1 Process Description and Model

The schematic diagram of divided wall column is given in **Figure 4-1**. It can be seen in the figure that the column has a single shell with a physical wall (movable or fixed and welded) partitioning it into the prefractionator and the main column. The column has six sections- C_{11} , C_{12} in the prefractionator and C_{21} , C_{22} , C_{23} , C_{24} in the main column. The reason for having six sections is that any configuration having less than six sections cannot produce reversible splits (Petlyuk, Platonoy and Slavinskii 1965). Also in each section, the components with highest and lowest boiling points should be separated in order to prevent mixing entropy (or to cause reversible splits) (Kaibel 1987). Each section in the column has twelve numbers of stages. The numbering of the stages used while stage by stage modeling of the column is shown in **Figure 4-1**. The equimolar feed consisting of three components (A, B and C) enters into the column at first stage of C_{12} . The basic column model is based on the same model as studied by Dwivedi et al. (Dwivedi, Halvorsen and Skogestad 2012). However the basic model's equations, input and output parameters were customized as per the requirement of this study.

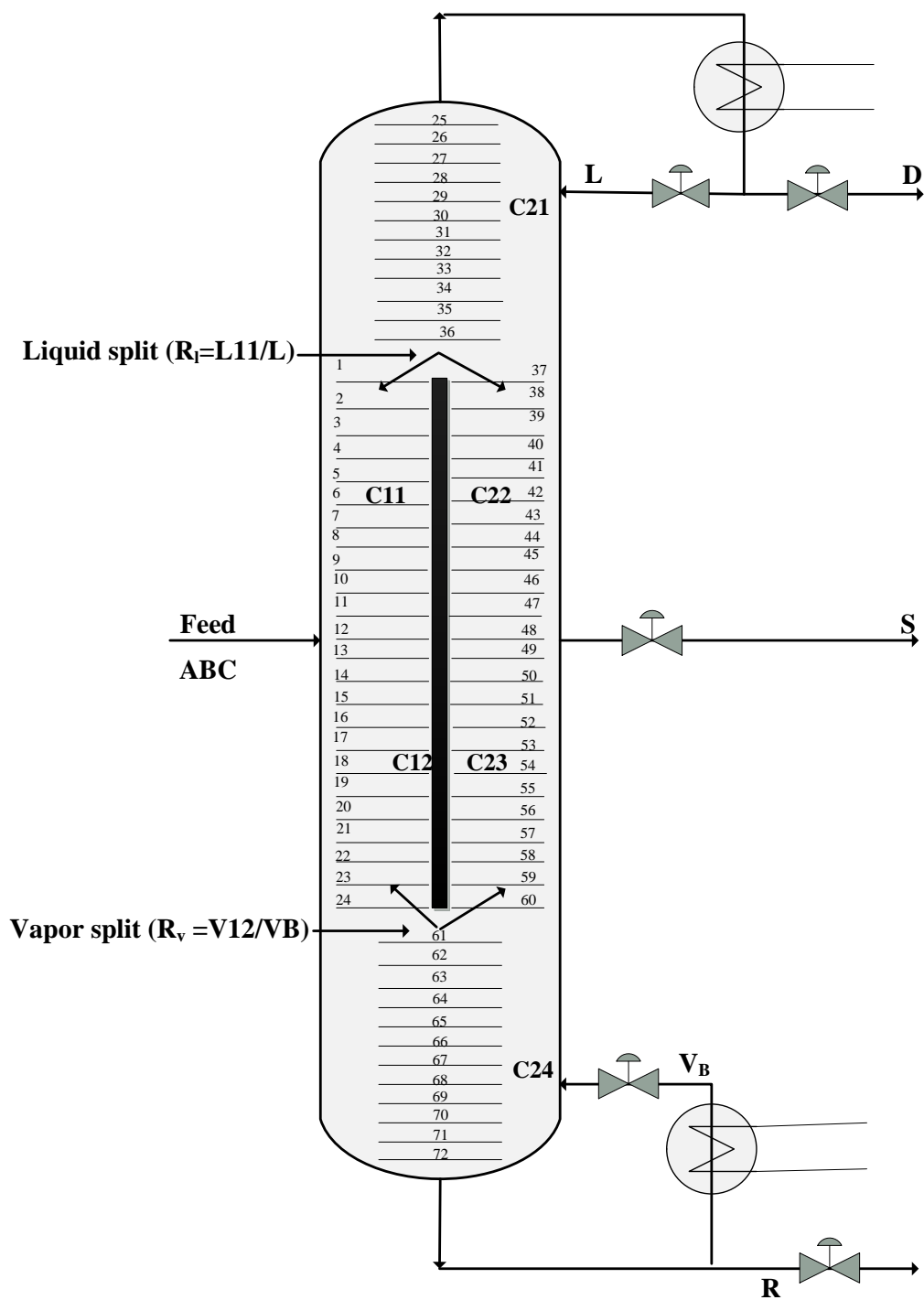


Figure 4-1: The schematic diagram of the three-product divided wall column

The stage by stage modeling of the column is based on following simplified assumptions:

- Constant relative volatility
- Constant Pressure
- Equilibrium on all stages
- Negligible vapor holdup
- Linearized Flow Dynamics
- Constant internal molar flows
- total condenser

The above assumptions are already explained in (**CHAPTER 2**). The column data with feed conditions and other process parameters are given in **Table 4-1**.

Table 4-1: Process data for the three-product divided wall column

Physical data	
Component A, B and C	Ethanol, Propanol and n-Butanol
Boiling points of A, B and C	[78.37 97 117.4]
Relative volatilities [A (lightest), B , C (heaviest)]	[4.2 2.1 1]
Number of stages	12 in each section
Nominal feed flow rate, F^*	1 [kmol/min]
Nominal feed composition, [z_A^* z_B^* z_C^*]	[0.333 0.333 0.333]
Nominal liquid feed, q_F^*	1
Disturbances (Deviations)	
Feed, F	$F^* \pm 10\%$
[z_A z_B]	[$z_A^* \pm 10\%$ $z_B^* \pm 10\%$]
V_{max}	$V_{max}^* \pm 10\%$
R_v	$R_v^* \pm 10\%$
Implementation errors	
Control error (integral action)	0.0000
Measurement error (temperatures)	± 0.5 °C

4.2 Plantwide Control Procedure for the Column

The step by step plantwide control procedure as discussed in section (3.1) of (CHAPTER 3) was applied to the control structure design of the three product divided wall column. The economic plantwide control procedure is for the implementation of optimal operation of the entire plant with many units and subunits. Here, the procedure is applied on the divided wall column while assuming it as a single unit of the plant. The procedure is discussed in the following subsections:

4.2.1 Define the Objective Function and the Constraints (DWC)

Based on the given model (stage-by-stage) assumptions for the three-product divided wall column, a typical scalar cost function subjected to various constraints is given below:

$$\min_{[x,u]} J = p_F F + p_V V - p_D D - p_S S - p_B B \quad (4.1)$$

F, V, D, S and B are flow rates (kmol/min) of feed, boilup, distillate, side stream and bottom product (residue) respectively. p_F, p_V, p_D, p_S and p_B are respective prices (\$/kmol) of flows. Usually, the modes of operation are defined based on the given feed condition (Mode-I, where energy usage is minimized or impurities in the products are minimized or a trade-off is established between two to maximize the profit). Mode-II is when feed is not given (in this case production is maximized, (S. Skogestad 2013))

In this study, Mode-I and Mode-II are based on the fact that whether the energy is expensive or cheap:

Mode-I: In this mode, energy is expensive therefore the optimal operation is subjected to minimizing the energy.

Mode-II: In this mode, energy is cheap therefore maximum energy can be used to maximize the profit from product recovery.

The objective function for this study has been deduced from **Eq. (4.1)** on the basis of following assumptions:

1. The given price of energy is cheap and therefore is fixed and is an active constraint (Mode-II)
2. Also the prices of each of the three products distillate (D), side stream (S) and bottom product R (R used as residue instead of B to avoid confusion with the component B) is dependent on the key component present in it.

$$p_D = p_A^0 x_{D,A}; \quad p_S = p_B^0 x_{S,B}; \quad p_R = p_C^0 x_{R,C}$$

Further, it is assumed that the unit price of each key component is same as given below:

$$p_A^0 = p_B^0 = p_C^0 = 1$$

Based on the assumptions (1 and 2) above, the cost function given by **Eq. (4.1)** can be rewritten as given below by **Eq. (4.2)**

$$\min_{[x,u]} J = x_{D,B}D + (x_{S,A} + x_{S,C})S + x_{R,B}R \quad (4.2)$$

The process constraints are:

Flow constraints: $\min \leq D, R, L \text{ etc.} \leq \max$

$$0 \leq D, R \leq F = 1$$

Column capacity (flooding): $V \leq V_{max}, V \leq 1.7319$

Pressure: P, given

Feed: F, given (d)

F is 1 Km/min

The constraints are also the non-negativity of states (compositions):

$$[u^T \quad x^T \quad d^T] \geq 0$$

where, u^T, x^T and d^T are input, compositions, holdups and disturbance vectors. The mode of operation is same as **Mode-II₀** in **Table 4-2**.

4.2.2 Optimization (Offline-Analysis, DWC)

In this step the degrees of freedom and expected disturbances at steady-state were identified and the optimization was done for disturbances. Also all possible modes of operations were identified based on the active constraints on the product purity specifications $x_{D,A}$, $x_{S,B}$ and $x_{R,C}$ and energy(V). These 4 constraints form 2^4 (16) different combination of active constraints. As earlier discussed in subsection 4.2.1, based on the energy economics, there are two modes of operation Mode-I and Mode-II. The possible modes of operation are given in **Table 4-2**.

Mode-II_{ABC} is not possible because all four constraints are active and thus controlled variables are more than the available degrees of freedom. Mode-I_{ABC} is same as minimizing energy for fixed product specifications. In this work **Mode-II₀**, which is same as minimizing the sum of impurities has been studied, **Eq. (4.2)**.

Table 4-2: Possible modes of operation for the three product divided wall column based on the active constraints

		Mode	No. of active composition constraints, $x_{D,A}$ in distillate D , $x_{S,B}$ in side stream S and $x_{R,C}$ in bottom product R			
			0	1	2	3
Energy Constraints	$V \leq V_{max}$	Mode-I Expensive Energy	Mode-I ₀ (1 case)	Mode-I _A /Mode-I _B / Mode-I _C , (3 cases)	Mode-I _{AB} /Mode-I _{BC} / Mode-I _{CA} , (3 cases)	Mode-I _{ABC} (1 case)
	$V = V_{max}$	Mode-II Cheap Energy	Mode-II ₀ (1 case)	Mode-II _A /Mode-II _B / Mode-II _C , (3 cases)	Mode-II _{AB} /Mode-II _{BC} / Mode-II _{CA} (3 cases)	(Infeasible)

The distillate flow rate D and bottom product flow rate R were used to control levels in the condenser and reboiler tank and also they do not have any effect on steady-state operation. The boilup $V(V_{max})$ and vapor split ratio R_v were assumed to be fixed and thus were not considered degrees of freedom rather they were assumed to be disturbances. The remaining degrees of freedom for optimization at steady-state are given below:

$$u^T = [L \ S \ R_L] \quad (4.3)$$

It was assumed that F was always a liquid feed i.e. $q_F = 1$ and so was excluded from disturbance vector d^T . The boilup and vapor split ratios are included in d^T .

$$d^T = [F \ z_A \ z_B \ V \ R_v] \quad (4.4)$$

Degrees of freedom Mode-II₀: In this mode there were no constraints on product purity specifications and only the constraint on the energy and vapor split ratio was active. The constraint on energy was active because it was assumed that energy was cheap and therefore it was set to be used at the maximum (V_{max}). The vapor split ratio was assumed to be constant because currently it is not common in practice to adjust it online however in few literatures it has been shown to be used as a manipulated variable.

4.2.3 Implementation of the Optimal Operation (DWC)

After identifying disturbances and input variables, the next step was to implement the optimal operation. For the implementation of optimal operation the active constraints are controlled first followed by unconstrained degrees of freedom. The constraints in this case study is active only on inputs boilup, V (V_{max}) and the vapor split ratio R_v as mentioned above. The candidate primary controlled variables for self-optimizing control were assumed to be the temperatures of stages in the column:

$$y^T = [T_1 \ T_2 \ T_3 \ \dots \ \dots \ \dots \ \dots \ \dots \ T_{71} \ T_{72}] \quad (4.5)$$

With six section and twelve stages in each of them, there were total seventy two candidate controlled variables available for self-optimizing control as given by **Eq.(4.5)**. Since, the objective function was to minimize the sum of impurities therefore the choice of compositions as the candidate controlled variables was ruled out. It is not advisable to select controlled variables which reach maximum or minimum at the optimum, (S. Skogestad 2000).

The methods for evaluating economic loss by using self-optimizing control in this study are given in **(CHAPTER 3)**.

4.2.4 Where to Set the Production Rate (DWC)

In this study, the boilup (V_{max}) was assumed to be the throughput manipulator because the feed was given and the only factor determining the production rate (product recovery here) was the boilup.

4.2.5 Regulatory Control Layer (DWC)

Regulatory control is usually meant for smooth and stabilized plant operation. In this study, the levels in the condenser (M_D) and the reboiler (M_B) were controlled by the distillate, D and bottom product flow rate, B respectively. The economic analysis for self-optimizing control was done on stabilized LV-model of the column.

4.2.6 Selection of Controlled Variables and Loss –evaluation (DWC)

The measurements or combinations of measurement chosen from the set of candidate controlled variables (temperatures on stages) were tested by evaluating loss for different value of measurement combination matrix H and $M(H)$ as given by **Eq.(3.21)**. In this work, the main emphasis is on calculating average loss as given by **Eq. (3.20)**, (Kariwala, Cao and Janardhanan 2008), where use of norm M to analyze the loss is known as “Exact local method”. However, (Kariwala, Cao and Janardhanan 2008) have used uniform distribution for d' and n^y , which results in an average loss of $\frac{1}{6(n_y+n_d)} \|M\|_F^2$, in this

work only, $\frac{1}{2}\|M\|_F^2$ has been used to calculate average loss. The steps involved in evaluating candidate controlled variables are briefly summarized below:

- Based on the optimal sensitivity and scaled gain matrix, the twenty best sets of temperatures were obtained using branch and bound algorithm, (Cao and Kariwala 2008).
- The worst case loss was calculated by using the formula given in **Eq. (3.23)** and also the loss was calculated for each set of temperatures using the respective values of their minimum singular value.
- Loss evaluation based on H matrix
 - (a) The average loss and worst case loss for above set of measurements as obtained from branch and bound method were also calculated using **Eq. (3.20)** and **Eq. (3.21)** by using the corresponding norm in *HY*.
 - (b) The average loss for H matrix obtained from null space method (without measurement noise)
 - (c) The average loss for H matrix using exact local method (with measurement noise)
- The loss caused by keeping first eight best sets of measurements (as obtained from branch and bound algorithm) constant as were also tested by simulating for change in disturbances using the non-linear model
- The loss caused by keeping the combinations of measurements as obtained from null space method were also tested by simulating for change in disturbances using the non-linear model
- The loss caused by keeping combinations of measurements as obtained by exact local methods was also tested by simulating for change in disturbances using the non-linear model.
- Finally the loss was evaluated for one case using the dynamic model

CHAPTER 5

Simulation Procedure

In the previous chapter the process and model of the system used in this work have been illustrated. Further, this chapter provides the information on retrieving the results obtained in this work. Major portion of this work like numerical computation, programming, modeling, simulations, optimization and control were done in MATLAB[®] R2101a.

5.1 Initialize the Steady-State Simulation

As earlier mentioned the work in this study was mainly focused on the control aspect of the three-product divided wall column therefore the stage by stage modeling of the column and assumptions for design conditions were generic and simple. Nevertheless the initial requirement emerged to be fixing the column design. The feed was considered to be an ideal liquid mixture consisting of three components A, B and C present in equimolar amount in it. The relative volatilities of the three given components happened to be same as those of Ethanol, Propanol and n-Butanol. Based on the feed conditions, V_{min} diagram was used to calculate the minimum energy required for operating the column and also the initial input variables to simulate the non-linear model (Halvorsen 2001) and (Halvorsen and Skogestad 1999)

5.1.1 Defining the Design Conditions

Minimum energy: For a given feed with three components A, B and C with constant relative volatilities, the minimum energy was found using Halvorsen's codes on V_{min} . The command to get the V_{min} plot is given in the beginning of the matlab code section. However one should download all codes (Halvorsen's code for V_{min}) in the same folder for using it. The minimum boilup value ($V_{min} = 1.3$ kmol/min) obtained from this

diagram is always for infinite number of stages and the peaks are for sharp product splits (i.e. zero impurity) and the most difficult split. The infinite number of stages means that the number of stages in section of the column is sufficient for sharp split between two components (heaviest and lightest). In this study it has been assumed that energy is cheap and the boilup is fixed at the maximum capacity of the column (V_{max}). The maximum value of boilup is limited by the flooding situation in column. The value of maximum boilup was assumed to be 30% higher than that of minimum boilup, ($V_{max} = 1.3V_{min}$).

Number of stages: The number of stages in each section of the column was assumed to be twelve. Based on previous studies by Dwivedi et al. (Dwivedi, Halvorsen and Skogestad 2012), simulation for the optimal operation (minimizing the sum of impurities) was initially done on the column with twenty numbers of stages in each section. Later on the numbers of stages in each section was brought down to twelve because with twenty numbers of stages in each section, the cost function was insensitive to change in inputs and disturbances.

Initial holdups: For this simple model, on each stage the normalized holdup of $M=1$ was assumed. However the holdups in condenser and reboiler tanks were assumed to be twenty times that of each stage.

Time: The time unit was not real and was assumed to be normalized time. The eigenvalues of the system, and the typical time constant directly depends on the holdup.

The non-linear model of the three-product divided wall column was created in Matlab. The models were based on the model studied by Dwivedi et al. (Dwivedi, Halvorsen and Skogestad 2012). The assumptions for the model have been already given in the previous chapter. The file to initialize the steady state simulation using ode solver is *init_runner.m*. It calls the non-linear model of the Petlyuk column *Petlyuk_NLmodel.m*. The script file *indmat_Yes_S1.m* has indices of all the states and hold ups. The divided wall column has six sections, first two sections in the prefractionator and remaining four sections in the main column. The prefractionator and the main column are in the same shell but

physically divided by a wall. The counting of stage starts from the top of the first section (C11) of the prefractionator and ends at the last section (C24) of the main column. Each stage has three states, two states for compositions and one state for hold up. The number of stages, relative volatilities, initial holdups and boiling point of three components are global values saved in the structures *coldata* and *dyndata*.

5.2 Optimization

The script file for running optimization is *Optimizer_Petlyuk.m* and the other related files are *specs.m* (linear equality and inequality constraints), *Petlyuk_nonlcon.m*. (nonlinear equality and inequality constraints) and *objective.m* (objective function). Optimization was done for minimizing the sum of impurities in the product streams and the solver used was *fmincon*. *Fmincon* solver is used to find the constrained minimum of function of several variables (Mathworks 2013). The optimal solutions obtained by running the optimization are saved in *Nominal_final.mat*. It has the nominal values of all states and holdups (*x_nom*) as well as inputs (*u_nom*). These values are made global by using global structure *dyndata* (*dyndata.x_nom*, *dyndata.u_nom* and *dyndata.temp_nom*).

5.3 Evaluation of Loss from Steady-state Linearized Model

The temperatures were chosen as candidate controlled variables because the objective function is to minimize the sum of impurities. According to Skogestad's palntwide control procedure (S. Skogestad 2000) one should never select the controlled variable which reaches maximum or minimum at the optimum. There were total seventy two temperatures which were assumed to be candidate controlled variables for implementing self-optimizing control structure. There were three degrees of freedom which could be manipulated to keep three controlled variables at constant setpoints. The measurements had to be chosen such that they would give acceptable loss when disturbances or implementation errors would shift the process away from optimum. The candidate controlled variables for self-optimizing control:

- Stage-temperatures in the prefractionator ($T_1 T_2 \dots \dots \dots T_{24}$)
- Stage-temperatures in the main-column ($T_{25} T_{26} \dots \dots \dots T_{72}$)

The output temperatures at the end of simulation or optimization can be obtained by calling the non-linear model function $[\text{sys Temp}] = \text{Petlyuk_NLmodel}(t,x,U)$. This function returns the derivatives and temperatures as output. The name of the function file is *Petlyuk_NLmodel.m*.

The initial nominal output temperatures have been saved as *Y0.mat*. Around this nominal point the model was linearized to obtain the optimal sensitivity matrix (F1), the input gain matrix (GY), the disturbance gain matrix (GYd), the second derivative of cost J (Juu) with respect to input and the second derivative of cost with respect to disturbances (Jud).

Optimal sensitivity from perturbation in disturbances: The script file to calculate optimal sensitivity is *Script_Fmatrix.m*. Also, the optimal sensitivity matrix is saved as *F1.mat*.

Gain Matrix from perturbation in inputs: The script file to calculate gain due to perturbation in inputs is *GYscript.m*. It is also saved as *GY.mat*.

Gain Matrix from perturbation in disturbances: The script file to calculate gain due to perturbation in disturbances is *GYdscript.m*. It is also saved as *GYd.mat*.

Juu and Jud matrix: Both the second derivatives of cost with respect to input and with respect to disturbances were calculated using central-finite-difference method and were also validated by forward and backward finite difference methods. The values are saved as *Juu.mat* and *Jud.mat*. Juu is a positive definite matrix.

Maximum minimum singular value: The script file to obtain sets of temperatures and respective maximum minimum singular values based on scaled gain G' is *min_singular.m*. It uses the function file *b3msv.m* which is based on the algorithm developed by (Cao and Kariwala 2008).

Bi-directional branch and bound for average loss criterion: The scripts file to calculate average loss for measurement subsets based on average loss criterion is

av_lossBB.m. It should be noted that it calculates the same loss as calculated by **Eq. (3.20)** and does not include $\frac{1}{6(n_y+n_d)}$ term. The function file *b3av.m* has been corrected to give same value as **Eq. (3.20)**.

Loss from null space method: The script file to get H matrix using null space method is *Nullspace_Petlyuk.m*.

Loss from exact local method: The exact local method gives good result only for very small value of disturbances and implementation errors. The script file used to calculate average loss and worst-case loss using exact local method for all combinations of measurements is *El_Petlyuk.m*. and for three measurements is *El_3Temp.m*.

5.4 Evaluation of Loss from Non-linear Model

The branch and bound method (Cao and Kariwala 2008) and bi-directional branch and bound method based on largest values of minimum singular values and the average loss criterion, (Kariwala, Cao and Janardhanan 2008) respectively gave best sets of three measurements. The five best sets of measurements (from maximum minimum singular value) giving minimum average loss were tested on the non-linear model. The loss was evaluated by keeping each set of measurements constant and changing each disturbance at one time. The changes were done in *Petlyuk_nonlcon.m* by adding these temperatures in non-linear equality constraints. *Plot_loss_MSV.m* is the script file for plotting loss.

Similarly the loss was plotted for both null space method and exact local method for change in feed. The script file is *plot_loss_nullspace.m*.

5.5 Evaluation of Loss from Dynamic Model

For the validation of steady-state simulation the set of controlled variables to be kept constant were also tested by dynamic simulation.

- Three individual measurement (T_{10}, T_{38}, T_{60}) obtained from maximum minimum singular value rule.

Step by step procedure for dynamic simulations:

The simulation files

1. The dynamic model was created with three inputs and three output loops controlled by proportional integrated controller (PI-controller). The name of the function file for non-linear dynamic model is *dynamic_Petlyuk.m*. It uses two function files *Petlyuk_NLmodel.m* (the steady-state non-linear model) and *Controller_PI.m* (function for PI controller action)
2. *Controller_PI.m* is a function file which has equations based on the proportional integrated control. The file has eight input variables and those are the output temperature (T), the setpoint temperature (T_s), the nominal input corresponding to the setpoint temperature (u_0), the integrated error (y), the controller gain (K_c), the integral time (τ_{ai}) and the valve opening limits (min,max).
3. *init_runner.m* is the script file to run the dynamic simulation. It has all the global parameters, the ode15s solver which takes initial states as inputs and returns the output states at the end of the simulation by solving the non-linear equations as given in the dynamic model.

The simulation procedure for self-optimizing control

1. Run the script file *init_runner.m* for initial simulation with no controller action by keeping all the loops open except two level loops closed as they are used in plant stabilization (regulatory control). And hence they are excluded from the self-optimizing control. The simulation would give the following results:
 - composition profiles in the prefractionator and the main column,
 - The mole fractions of components A, B and C in the product streams of the main column (D,S and R) as well as the prefractionator (D,S and R1)
 - The cost which is the total sum of impurities in the products coming out from the main column.
2. The second important step of the procedure was to tune the PI controller. Since, there were three input variables (DOF) and three output variables (Temperatures on stages) therefore the sequential tuning method (Hovd and Skogestad, Sequential Design of Decentralized Controllers 1994) was used. In the sequential

tuning method, firstly, the prefractionator was tuned independently and then the PI controller loops in the main column were tuned one by one starting from the reflux followed by the side-stream.

3. The step change was given in the nominal input value of liquid split ratio R_1 (dyndata.u_nom(3)) and the step response was seen in the output temperature T_{10} (temperature corresponding to 10th stage of the column in the prefractionator, Temp_current(3)). The response was same as for the integrating process with small dead time, θ . The tuning parameter K_c and integral time τ_I were identified for the process and the loop was closed to see the response with setpoint change and the disturbances.
4. After tuning the input –output loop R_1 and T_{10} in the prefractionator the next step was to tune reflux L (kmol/min) with the output temperature T_{38} . The step change was given in the nominal input value of reflux flow rate L (dyndata.u_nom(2)) and the step response was seen in the output temperature T_{38} (temperature corresponding to 38th stage of the column in the main column, Temp_current(1)). The response was same as for the integrating process with small dead time, θ . The tuning parameter K_c and integral time τ_I were identified for the process and the loop was closed to see the response with setpoint change and the disturbances.
5. After tuning the input –output loop S and T_{60} in the main column the last step was to tune side stream flow rate S (kmol/min) with the output temperature T_{60} . The step change was given in the nominal input value of reflux flow rate S (dyndata.u_nom(5)) and the step response was seen in the output temperature T_{38} (temperature corresponding to 60th stage of the column in the main column, Temp_current(2)). The response was same as for the integrating process with small dead time, θ . The tuning parameter K_c and integral time τ_I were identified for the process and the loop was closed to see the response with setpoint change and the disturbances.
6. After tuning all three loops they were closed in order to validate the results of self-optimizing control obtained from the steady-state simulation. For change in disturbances from the nominal the costs were obtained from dynamic simulations.

The changes in disturbances were done to obtain loss evaluation using self-optimizing control structure.

Table 5-1: SIMC tuning parameters used in the self-optimizing control structure

Control loop	K_c	τ_I
<i>R_l</i>	-0.33	8
<i>L</i>	-0.15	16
<i>S</i>	0.27	11.2

CHAPTER 6

Results and Discussion

The method for selection of controlled variables for self-optimizing control has been already discussed in Chapter 3. Also, how these methods were implemented on the three-product divided wall column has been elaborated in (CHAPTER 4). Further, the procedure for simulation using these methods to generate results has been discussed in (CHAPTER 5). All possible modes of operation are given in Table 4-2. In this chapter, the results and discussions for Mode-II₀ has been presented.

6.1 Initial Steady-State Simulation

6.1.1 Defining the design conditions

The data for the column design like feed flow rate, feed conditions, number of stages in the column are given in Table 4-1. The graphical (V_{min}) diagram was used to find initial inputs for the column with a given feed.

Minimum energy (V_{min}) and maximum boilup (V_{max}): In this study, the column has been assumed to be operating at the fixed maximum boilup. The maximum boilup V_{max} was assumed to be 30% higher than the minimum boilup V_{min} . The minimum energy required to operate the column can be found by using graphical V_{min} diagram proposed by Halvorsen (Halvorsen 2001). The minimum energy required to separate the multi component feed is equal to the most difficult binary separation (Halvorsen and Skogestad 2003). The factors affecting the value of V_{min} are feed flow rate, feed composition, feed liquid composition and the relative volatilities of feed components.

For an equimolar feed with given relative volatilities the split was more difficult between component B and C. However, with an increase in component A and decrease in

component B in the feed the split was more difficult between components A and B, **Figure 6-1**. The minimum energy for this study from graphical V_{min} diagram was found to be 1.3 (kmol/min). This is because B and C split has the highest peak (V/F). The value of minimum boilup (1.3 kmol/min) was based on the assumptions that there were sufficient numbers of stages in each section of the column for sharp separation between the components.

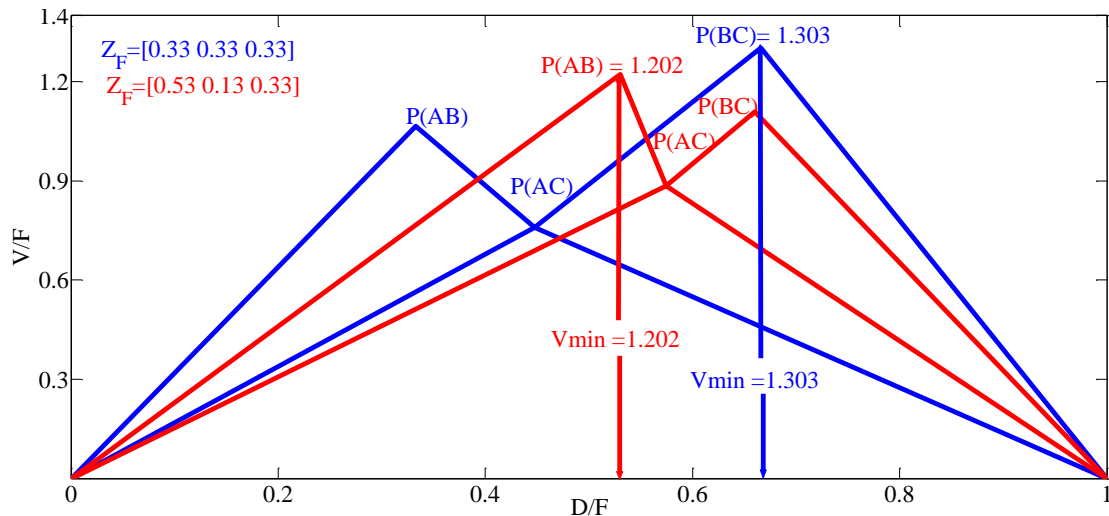


Figure 6-1: V_{min} diagrams for two different compositions of feed with relative volatilities, $\alpha = [4.2 \ 2.1 \ 1]$

The value of maximum boilup ($V_{max} = 1.7319$) to be used for this study was made 30% higher than that from the minimum energy.

Number of stages: There were approximately twenty numbers of stages corresponding to the minimum energy that would give sharp separation. The cost function was equivalent to minimizing the sum of impurities for fixed and maximum boilup. The cost function with twenty numbers of stages and given maximum boilup was apparently insensitive to changes. Therefore, the number of stages was reduced to twelve in each of six sections of the column.

Steady-state simulation: The initial composition (x) on all stages were assumed to be 0.333 and simulation was done to obtain new steady-state values. The new steady-state

values are given in **Table 6-1** and **Table 6-2**. The total sum of impurities in products at the new steady-state was 0.2077 (kmol/min). The sum of impurities at the steady-state was very high. Optimization was done to bring down the sum of impurities and find the nominal conditions for the column operation.

Table 6-1: Input values used for initial steady-state simulation with 12 stages in each section

Reflux flow rate, L	1.0033 (kmol/min)
Boilup flow rate, V	1.3381 (kmol/min)
Liquid split ratio, R_l	0.3465
Vapor split ratio, R_v	0.5982
Distillate flow rate, D	0.3348 (kmol/min)
Side stream flow rate, S	0.3318 (kmol/min)
Bottom Product, R (R is used instead of B)	0.3333 (kmol/min)

Table 6-2: Compositions at steady-state in the main column and the prefractionator of the column

Product Streams	Compositions		
	x_A	x_B	x_C
Distillate, D	0.9867	0.0133	0.0000
Side product, S	0.0089	0.9710	0.0201
Bottom product, R	0.0000	0.0201	0.9799
Prefractionator top product, $D1$	0.4148	0.5675	0.0177
Prefractionator bottom product, $R1$	0.0117	0.6037	0.3845

6.2 The Nominal Values from Optimization

The optimization was done with respect to degrees of freedom and for the cost function as given below in **Eq. (6.1)**:

$$J = Dx_{D,B} + S(x_{S,A} + x_{S,C}) + Bx_{R,B} \quad (6.1)$$

The cost function as given above is the total sum of impurities in product streams coming out of the main column. The unconstrained degrees of freedom for self-optimizing control are reflux flow rate, side stream flow rate and the liquid split ratio as given below:

$$u^T = [L \ S \ R_L] \quad (6.2)$$

There are five disturbances and they are feed flow rate, composition of A and B in the feed, the boilup which is fixed and set at the maximum and the vapor split ratio, **Eq.(6.3)** :

$$d^T = [F \ z_A \ z_B \ V \ R_V] \quad (6.3)$$

Optimization was done with steady-state values as initial values and the results for optimization are presented in **Table 6-3** and **Table 6-4**. The optimization was done several times to ensure the minimum cost. The nominal value of sum of impurities came out to be 0.0037(kmol/min). The nominal values of fraction of impurities A and C in the prefractionator bottom and top were 0.0029 and 0.0015. These values seemed to be relatively good for feasible composition profiles in both the prefractionator and the main column.

Table 6-3: The input values at the nominal conditions for DWC

Reflux flow rate, L	1.3986 (kmol/min)
Boilup flow rate, V	1.7319 (kmol/min)
Liquid split ratio, Rl	0.3834
Vapor split ratio, Rv	0.5874
Distillate flow rate, D	0.3382 (kmol/min)
Side stream flow rate, S	0.3332 (kmol/min)
Bottom Product, R (R is used instead of B)	0.3329 (kmol/min)

Table 6-4: Product compositions in the main column and the prefractionator of DWC

Product Streams	Compositions		
	x_A	x_B	x_C
Distillate, D	0.9970	0.0030	0.0000
Side product, S	0.0033	0.9938	0.0029
Bottom product, R	0.0000	0.0018	0.9982
Prefractionator top product, D1	0.4066	0.5905	0.0029
Prefractionator bottom product, R1	0.0015	0.5749	0.4236

The nominal composition and temperature profiles in the prefractionator and the main column are given in **Figure 6-2** and **Figure 6-3**. The temperature profiles in both the

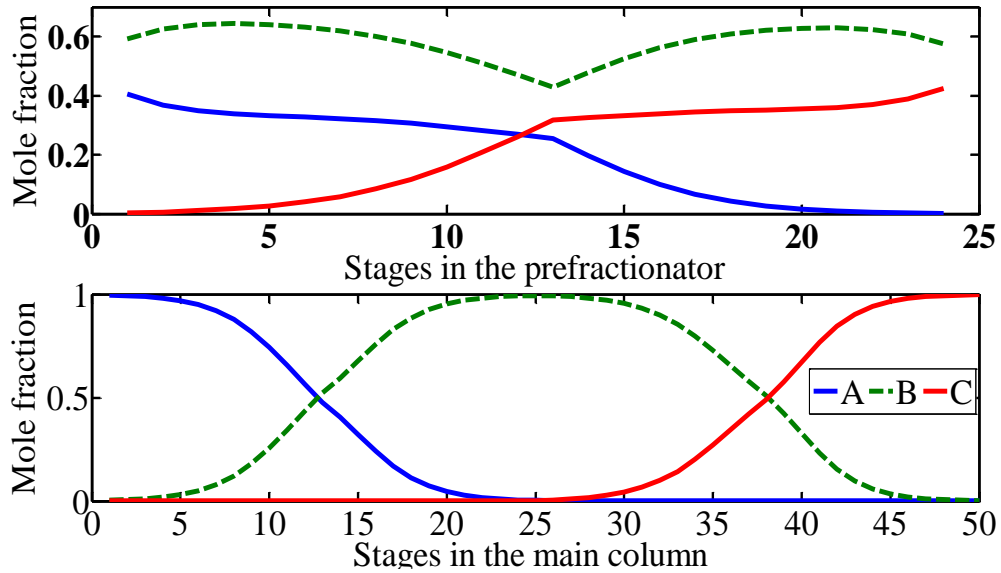


Figure 6-2: Optimal composition profiles in the prefractionator and the main column respectively of the three-product divided wall column

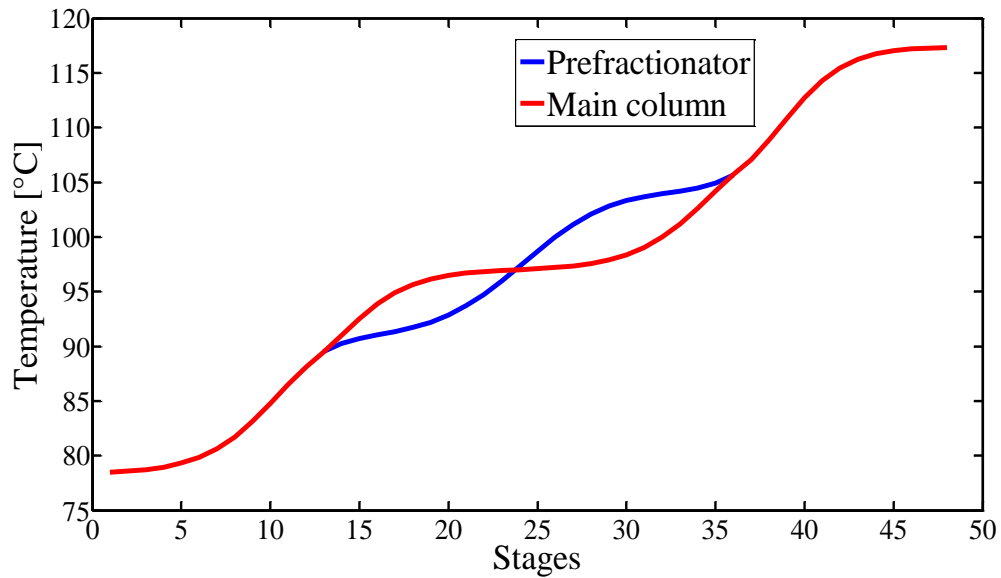


Figure 6-3: Optimal temperature profile in the three-product divided wall column

prefractionator and the main column are shown in the same figure. Stages (1-24) of the prefractionator share the common height with the main column's stages (13-36). The temperature profile in the column shows increase in stages temperature from top towards bottom both in the prefractionator and the main column. This is usual because of the heating from reboiler in the bottom of the column.

6.3 Re-optimized values with disturbances

Re-optimization was done for expected disturbances in future and the effect was seen on the cost. The deviation in disturbances from nominal is already given in section (4.1.) The variation in cost with respected to deviation in disturbances are given in **Table 6-5**. The resulting cost went up with increased value of disturbances (10% higher from the nominal) except when boilup flow rate was increased. This is as expected because the increase in energy would result into more pure products. The resulting optimal cost due to decrease in disturbances (except boilup) was even lower than that from the optimal cost.

The values of re-optimized cost given in **Table 6-5** are not very accurate and the cost might have gone further down on re-optimizing nevertheless it can be assumed that these values are very close to optimal values at the respective values of disturbances. The actual re-optimized cost with respect to disturbance might only be 1-5% lower than the current values given in **Table 6-5**.

Table 6-5: The re-optimized cost with respect to expected future disturbances

Disturbances	Cost		
	$J(d^*)$	$J(d^*) + 10\%$	$J(d^*) - 10\%$
F	0.0037	0.0061	0.0023
z_A	0.0037	0.0041	0.0035
z_B	0.0037	0.0043	0.0031
V_{max}	0.0037	0.0026	0.0059
R_v	0.0037	0.0043	0.0036

6.4 Loss Evaluations using Pseudo/Steady-state Linearized Model

The candidate controlled variables were temperatures on each stage of the column and they are given in (CHAPTER 4) and (CHAPTER 5). The average loss and worst-case loss was evaluated using different measurement combination matrix H obtained from maximum minimum singular rule (Cao and Kariwala 2008) , bi-directional branch and bound method based on the average loss criterion (Kariwala, Cao and Janardhanan 2008), exact local method (minimum loss method) and null space method. The formula for average loss evaluation was same as used recent literature by Yelchuru and Skogetsad, (Yelchuru and Skogestad 2012) and is given by **Eq. (3.20)** and **Eq. (3.21)**.

6.5 Results from Maximum Minimum Singular Rule

In this case study, the total numbers of candidate controlled variables were seventy two and for self-optimizing control only three measurements or three sets of combinations of measurements were needed because there were only three unconstrained degrees of freedom. Using the brute force method to check the candidacy of each of the available measurements (72 temperatures) was tedious task. In order to make the task simpler and to select the best set of three temperatures the maximum minimum singular value rule was applied.

6.5.1 Optimal Sensitivities

The pseudo/steady-state loss evaluation methods used in this study require the calculation of optimal sensitivity of the output (temperatures) with respect to disturbances. The optimal sensitivity F ($F1$ in this study) was obtained directly from its definition, i.e. $F = \frac{dy_{opt}}{dd}$. Plots of optimal sensitivity with respect to each disturbances ($V, F, z_A, z_B,$ and R_v) are shown in **Figure 6-4, Figure 6-5, Figure 6-6, Figure 6-7 & Figure 6-8**. The requirement of a good self-optimizing controlled variable is that its value should not be sensitive to disturbances, (S. Skogestad 2000).

Figure 6-4 shows the optimal sensitivity of output temperatures with respect to change in boilup both in the prefractionator and the main column. The optimal variation in output temperatures in this case is mainly in the bottom of the column. The effect of

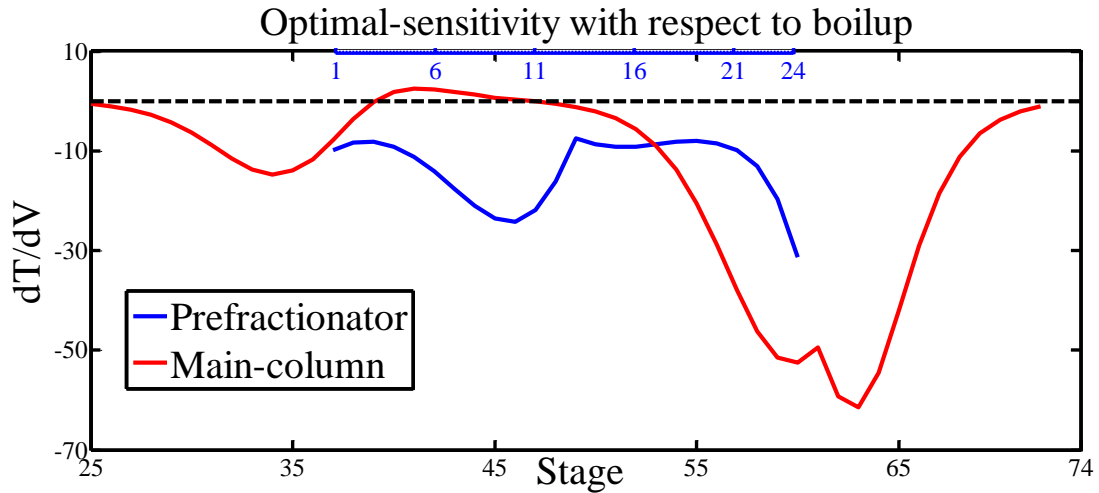


Figure 6-4: Optimal-sensitivity of output temperatures with respect to the boilup

change in disturbance (boilup) is mainly in the vapor split zone in both the main column(63rd stage) and the prefractionator (24th stage).

Figure 6-5 shows the optimal sensitivity of output temperature of the prefractionator and main column due to feed flow rate. The variation in the temperature can be seen mainly at the both ends of the prefractionator. In the main column, the variation in output temperatures is mainly in the vapor and liquid splitting sections.

The sharp variation in optimal sensitivity of output temperatures near feed stage in the prefractionator is clearly visible in the **Figure 6-6**. It seems that the effect of the disturbance in the composition A in feed has effect in the vapor split zone in the main column and that has caused sharp temperature variation near vapor split stage in the main column.

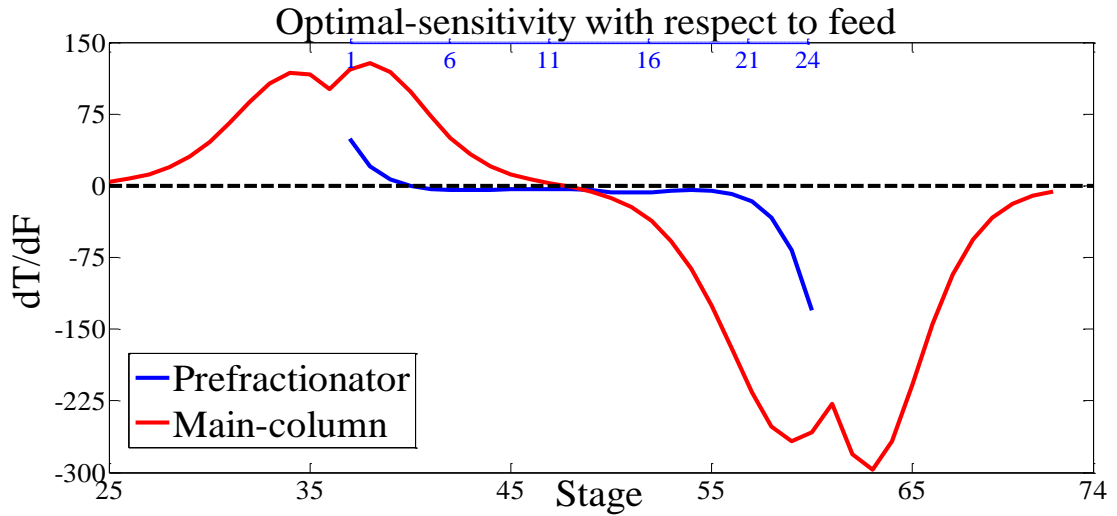


Figure 6-5: Optimal-sensitivity of output temperatures with respect to the feed

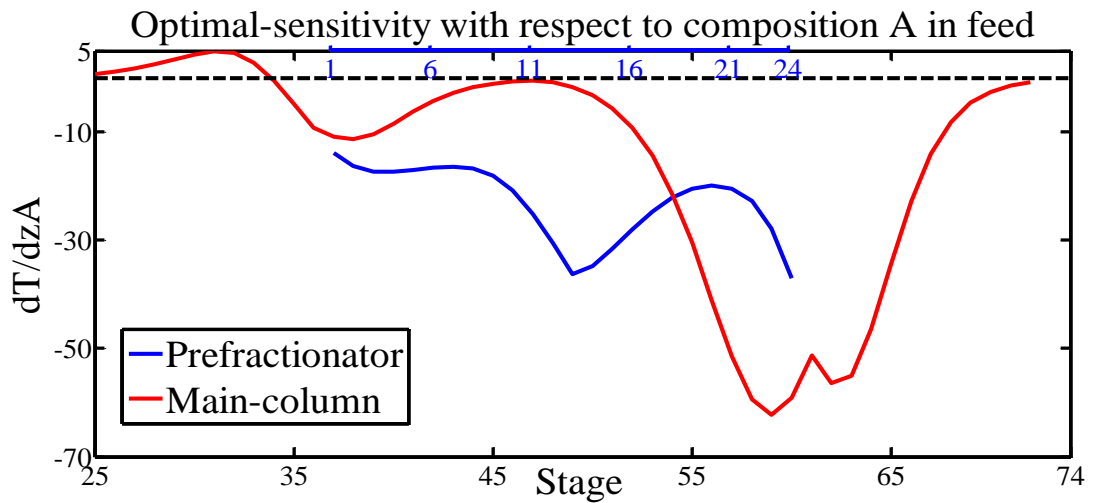


Figure 6-6: Optimal sensitivity of output temperatures with respect to composition of A in the feed

Similarly, **Figure 6-7** shows the change in optimal sensitivity of the output temperatures (due to composition B in feed) in the prefractionator is large near the feed section. The effect in the main column is near the vapor split and liquid split zones.

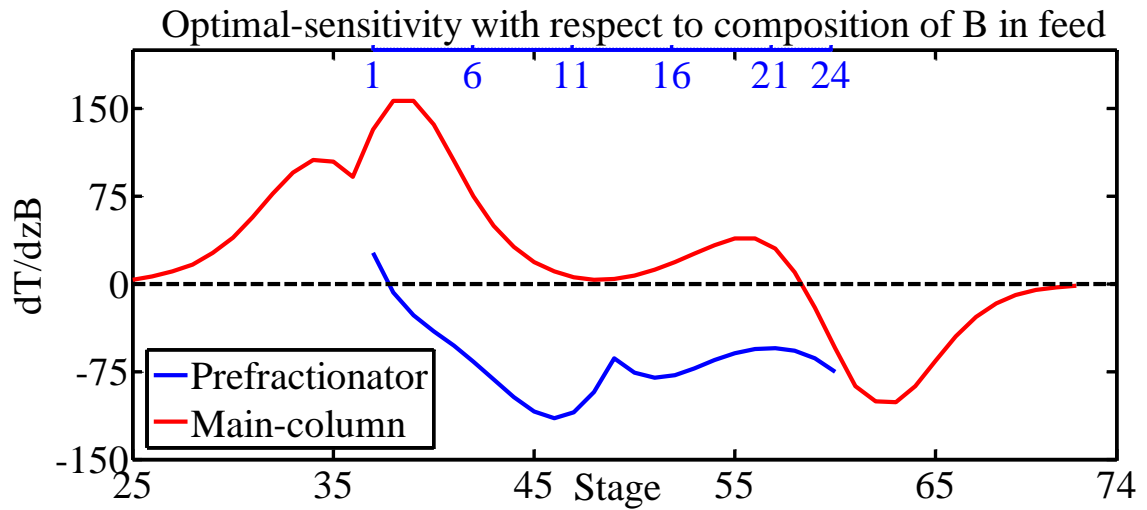


Figure 6-7: Optimal-sensitivity of output temperatures with respect to composition of B in the feed

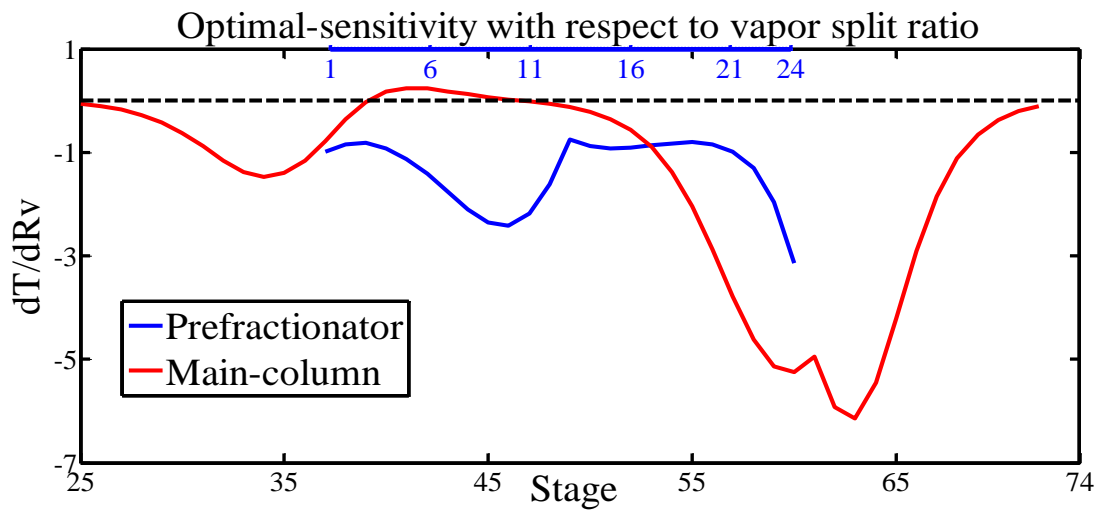


Figure 6-8: Optimal-sensitivity of output temperatures with respect to the vapor split ratio

The optimal sensitivity of output temperatures with respect to change in vapor split ratio has been plotted in **Figure 6-8**. The sharp variation in the temperature change near vapor

split is clearly visible in the figure. It seems that the effect of the vapor split in the main column has impact on the stage near liquid split zone. It might be due to the variation of the vapor and liquid flow rates in the prefractionator and the main column.

6.5.2 Scaled Gain

The scaled gain of output temperatures from the individual inputs, the reflux flow rate, the side stream flow rate and the liquid split ratio respectively are shown in **Figure 6-9**.

The candidate controlled variables showing relatively higher gain are assumed to be

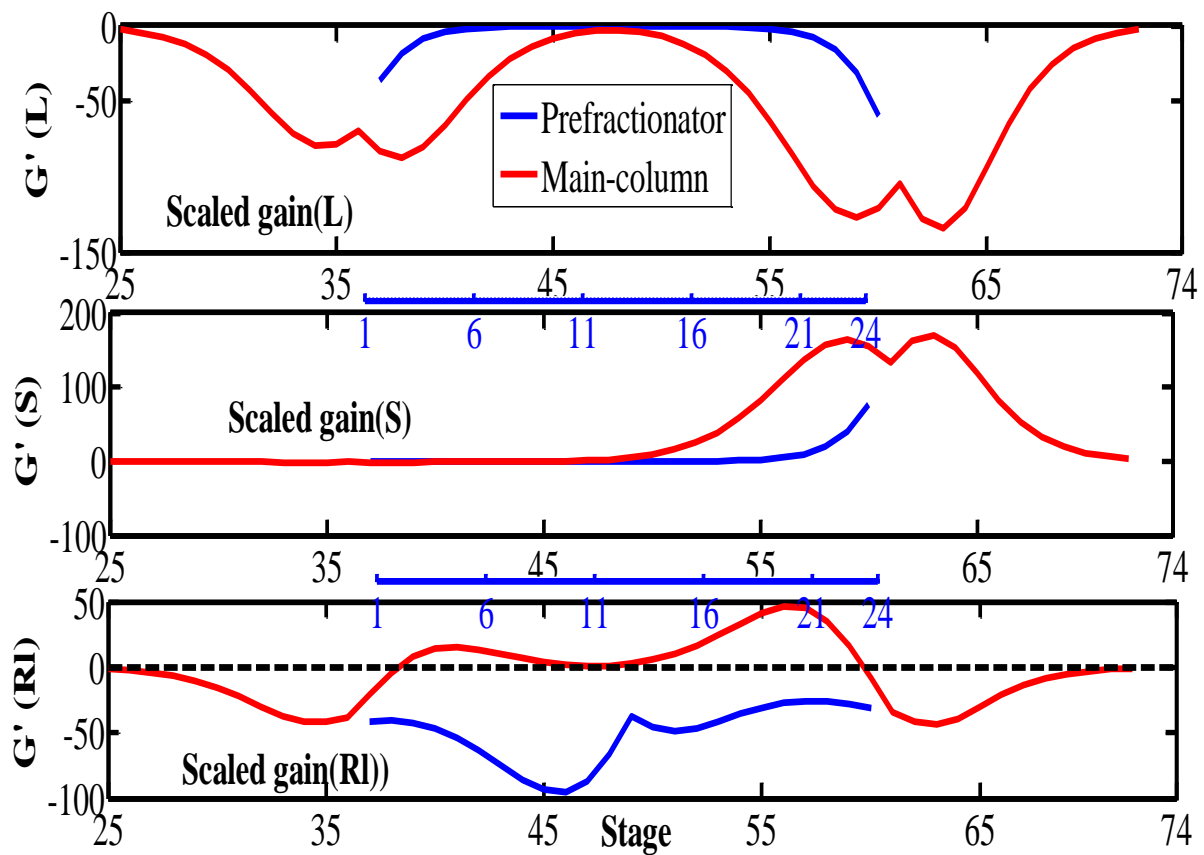


Figure 6-9: Scaled gains in the prefractionator and the main column for unconstrained degrees of freedom

better controlled variables (S. Skogestad 2000). In the prefractionator, maximum gain can be seen on 10th stage for change in input variable R_i . Similarly, in the main column the highest gain is seen on 63rd stage (section-C₂₅) and 38th stage (section-C₂₂). With change in input S, the maximum gain is again seen on 63rd stage (section-C₂₅). Thus, based on scaled gain, these stages (T₁₀, T₃₈ and T₆₃) can be considered to be good candidate controlled variables for self-optimizing control.

After finding the scaled gain G' as prescribed in (**CHAPTER 3**), the worst-case loss was calculated to be:

$$L_{wc} = 0.0029$$

In order to minimize the worst case loss as found above, those controlled variables were selected which would give the maximum minimum singular value for the scaled steady-state gain G' .

The branch and bound algorithm by Cao and Kariwala (Cao and Kariwala 2008) was used to find the ten best sets of measurements. Each set contained three measurements (stage temperature here) equivalent to the number of available degrees of freedom for self-optimizing control. **Table 6-6** shows ten best set of temperatures with their ranking in decreasing order. The set with the highest value of minimum singular value was assumed to be the best set of measurements to be kept constant for self-optimizing control at the steady-state. The best set of three temperatures based on the highest value of minimum singular value is:

$$c_y^T = [T_{10} \ T_{38} \ T_{60}] \quad (6.4)$$

The corresponding minimum singular value for the above mentioned best set of temperatures came out to be:

$$\underline{\sigma}(G_s) = 67.155 \quad (6.5)$$

Table 6-6: Ten best sets of temperature as candidate controlled variables based on maximum minimum singular value rule

Rank	CV ₁	CV ₂	CV ₃	$\underline{\sigma}(G_s)$	Loss(10^{-4})
1	10	38	60	67.155	1.1087
2	9	38	60	67.152	1.1088
3	11	38	60	67.152	1.1088
4	10	38	63	67.143	1.1091
5	8	38	60	67.135	1.1094
6	9	38	63	67.128	1.1096
7	7	38	60	67.035	1.1127
8	10	38	59	66.970	1.1149
9	10	38	62	66.945	1.1157
10	11	38	63	66.945	1.1157

The value of loss as calculated above using **Eq. (3.21)** is relatively less accurate than the loss calculated by **Eq.(3.19)** and **Eq.(3.20)**. This is because the loss calculation using scaled gain requires appropriate scaling of inputs and outputs and selecting an exact scaling is difficult because of many possible numbers of combinations of disturbances and implementation errors. In the next section, loss evaluation is done using local method which use H and $M(H)$ matrices and give more accurate results.

6.6 Loss Evaluation using H matrix (Local Methods)

The theory related to local methods is illustrated in (**CHAPTER 3**), here these methods have been used to evaluate and identify the promising CVs for self-optimizing control. The losses were evaluated based on the H matrix for individual measurements and the combinations of measurements.

6.6.1 Loss Evaluation with three Measurements

New ranking of sets obtained from maximum minimum singular value: The average loss and worst case loss was calculated using the H matrix for 10 best sets of temperatures as given in **Table 6-6**. On calculating the average loss it was found that the ranking of the best set of measurements as calculated by branch and bound method based on maximum minimum singular value in **Table 6-6** was changed and **Table 6-7** shows new ranking based on the values of average loss.

Table 6-7: Average loss and worst-case loss for 10 best sets of measurements (here, $n_y = n_u$) using minimum loss method

Rank	CV ₁	CV ₂	CV ₃	$\frac{1}{2} \ M\ _F^2$ (10 ⁻⁴)	$\frac{1}{2} \bar{\sigma}(M)^2$ (10 ⁻⁴)
3	10	38	60	9.63	7.781
2	9	38	60	9.61	7.780
5	11	38	60	9.784	7.777
8	8	38	60	1.001	8.137
4	10	38	63	9.687	7.776
7	9	38	63	9.994	8.135
6	7	38	60	9.866	7.770
1	10	38	59	9.430	7.604
10	10	38	62	1.399	8.337
9	9	38	62	1.019	8.135

The best set of three temperatures based on the minimum value of average loss as calculated by using **Eq. (3.20)** and **Eq.(3.21)** is:

$$c_y^T = [T_{10} \ T_{38} \ T_{59}] \quad (6.6)$$

The best set of stage temperatures obtained from **Eq. (6.4)** and **Eq.(6.6)** were almost same with respect to their positioning in the column's section. Also, there was not much difference in the positioning of the stage's temperatures for first three best sets of measurement obtained in **Table 6-6** and **Table 6-7**. The best sets of temperatures as given by **Eq. (6.4)** and **Eq. (6.6)** seem to be good from the regulatory control point of view as well. The reasons being it is that they were in three different sections of the column and each of these sections was close to one of the available unconstrained degrees of freedom. Based on intuition the following pairing can be made between the controlled variable and the manipulated variables (here, unconstrained degrees of freedom):

$$R_l \leftrightarrow T_{10} \quad (6.7)$$

$$L \leftrightarrow T_{38}$$

$$S \leftrightarrow T_{59} \text{ or } T_{60}$$

The above pairing can be made for self-optimizing control to meet the economic objective which is minimizing the sum of impurities here. The above pairing can also be used for regulatory control in order to stabilize the column dynamically but the steady-state RGA (relative gain array) analysis should be done to avoid wrong pairing with close interactions in decentralized control structure. The regulatory control based on RGA analysis has been presented in the later section of this report.

New ranking of sets obtained from bi-directional branch and bound method based on average loss criterion: The bidirectional branch and bound method for average loss criterion gave 10 different sets of temperatures as the best candidate controlled variables as given in **Table 6-8**. The best sets of temperature in this case are also similar to the sets of temperatures obtained in **Table 6-6** and **Table 6-7** except set of temperatures with rank 4. The positioning of set of temperatures with rank 4 is different from other sets of available measurements based on ranking.

In **Table 6-8**, two of the columns are presenting the values of average loss corresponding to each sets of temperature. L_{avg} is the average loss calculated by bi-directional branch and bound algorithm however $\frac{1}{2} \|M\|_F^2$ is the average loss calculated

Table 6-8: Average loss and worst-case loss for ten best sets of measurements (here, $(n_y = n_u)$) using bidirectional branch and bound method, (Kariwala, Cao and Janardhanan 2008)

Rank	CV ₁	CV ₂	CV ₃	L_{avg} 10 ⁻³	$\frac{1}{2} \ M\ _F^2$ 10 ⁻⁴	$\frac{1}{2} \bar{\sigma}(M)^2$ 10 ⁻⁴	
1	9	38	59	1.17	9.41	7.60	4
2	9	38	58	1.17	9.31	7.50	1
3	9	39	59	1.17	9.43	7.61	5
4	39	57	63	1.17	1.00	7.64	9
5	9	39	58	1.17	9.32	7.50	2
6	8	38	59	1.18	9.49	7.61	7
7	10	38	59	1.18	9.50	7.61	8
8	8	38	58	1.18	9.39	7.51	3
9	8	39	59	1.18	9.39	7.51	3
10	10	39	59	1.18	9.44	7.61	6

based on the value of H and norm of $M(H)$ from exact local method (minimum loss method). It should be noted that L_{avg} in **Table 6-8** was calculated after making correction in the term $(\frac{1}{6(n_y+n_d)})$ (matlab codes) and therefore both the values of L_{avg} and $\frac{1}{2}\|M\|_F^2$ should have been nearly same.

Summary: The average loss was calculated for first 10 best sets of measurements. The ranking of these measurements was based on

- maximum minimum singular value calculated from branch and bound method (Cao and Kariwala 2008)
- bi-directional branch and bound method for average loss criterion, (Kariwala, Cao and Janardhanan 2008)

For the sets of measurements calculated from both methods mentioned above the average loss was calculated using H and norm of $M(H)$ matrix as given in recent literature, (Yelchuru and Skogestad 2012) and new ranking was made. It was found that the bi-directional branch and bound method gives different value of average loss and therefore should be investigated in further work. The three best sets of temperatures obtained from these methods are nearly same in terms of values of average loss as well as the positioning in the column's stage. These sets of temperatures seem good candidate controlled variables for self-optimizing however further validation can be done for larger disturbances on non-linear model.

6.6.2 Loss Evaluation (Exact Local Method)

The H matrix as calculated from exact local method (minimum loss method) gives the average loss as given below:

$$L_{avg} = \frac{1}{2}\|M\|_F^2 = 7.5166 \times 10^{-4} \quad (6.8)$$

and the worst case loss using H matrix from exact local method is :

$$L_{wc} = \frac{1}{2} \overline{\sigma}(M)^2 = 6.6486 \times 10^{-4} \quad (6.9)$$

The values of both average loss and worst-case loss in this case are less than those for values given in **Table 6-7** and **Table 6-8**. This is as expected because here all combinations of measurements were kept at constant setpoints whereas the loss values in **Table 6-7** and **Table 6-8** are obtained by keeping only three temperatures at constant setpoints at a time. Increase in numbers of measurements in H matrix averages out the measurement noise while calculating loss.

6.6.3 Loss Evaluation (Null Space Method)

Since, the number of available measurements (temperatures on all stages, $n_y = 72$) is greater than the sum of the degrees of freedom and disturbances ($n_u + n_d = 3 + 5 = 8$), therefore neglecting the measurement noise, (i.e. $W_{ny} = 0$), gave the measurement combination matrix H calculated from exact local method equivalent to that from null space method and the loss is given by:

$$L_{avg} = \frac{1}{2} \|M\|_F^2 = 1.4491 \times 10^{-25} \cong 0 \quad (6.10)$$

and the worst case loss using H matrix from null space method is also approximately zero :

$$L_{wc} = \frac{1}{2} \overline{\sigma}(M)^2 = 1.4491 \times 10^{-25} \cong 0 \quad (6.11)$$

6.7 Loss Evaluation from Non-linear Model

Local methods are used to prescreen the most promising CVs based on the values of average loss and are based on the pseudo/steady-state linear model. This method takes relatively very less CPU time than evaluating loss from other methods based on non-linear model especially when available measurements are very large in numbers. Also these methods give less loss for small change in disturbances. In case of large

disturbances the non-linearity in the model might not give good results. Based on the values of average loss (L_{avg}) as given in **Table 6-7** and **Table 6-8**, it was found that the bi-directional branch and bound method gives lesser values of losses for all sets of measurements except one set (new rank 9 in **Table 6-8** and new rank 1 in **Table 6-7**). The values of worst-case loss are also comparatively better than that from sets of measurements obtained using maximum minimum singular rule. Based on pseudo/steady-state analysis, it can be concluded that the bidirectional branch and bound method gives better sets of measurements for self-optimizing control than the branch and bound method using maximum minimum singular values. The first five sets of candidate controlled variables based on the bi-directional branch and bound algorithm by (Kariwala, Cao and Janardhanan 2008) are :

$$c_y^T = \begin{bmatrix} T_9 & T_{38} & T_{58} \\ T_9 & T_{39} & T_{58} \\ T_8 & T_{38} & T_{58} \\ T_8 & T_{39} & T_{59} \\ T_9 & T_{39} & T_{59} \end{bmatrix} \quad (6.12)$$

The sets of measurements given by **Eq. (6.12)** should have been tested on non-linear model by keeping each temperature in each set constant by varying one disturbance at a time. The evaluation of loss by this method is called brute force method.

The loss evaluation using brute force method could not be tested for the measurements given in **Eq. (6.12)** because of lack of time. However the loss evaluation using brute force method was already done for the first five best sets of values obtained in **Table 6-7** and is also presented here. The candidate controlled variables which were evaluated by brute force method on non-linear model for larger disturbances are:

$$c_y^T = \begin{bmatrix} T_{10} & T_{38} & T_{59} \\ T_9 & T_{38} & T_{60} \\ T_{10} & T_{38} & T_{60} \\ T_{10} & T_{38} & T_{63} \\ T_{11} & T_{38} & T_{60} \end{bmatrix} \quad (6.13)$$

The loss is plotted for only change in feed flow rate.

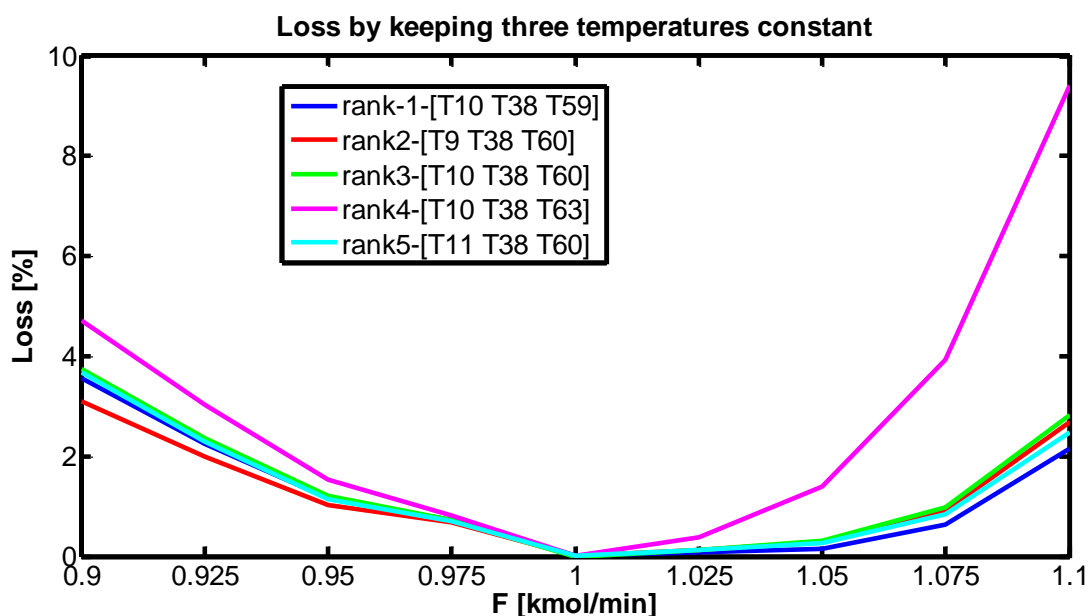


Figure 6-10: The loss obtained from the non-linear model due to disturbance in feed flow rate for self-optimizing control by keeping three temperatures constant

The candidate controlled variables in **Eq.(6.13)** were found to be first five best sets of temperatures based on the average loss calculation using local minimum loss method as given by **Eq. (3.20)** and **Eq. (3.21)**. Those sets of measurement were also tested on the non-linear model of the column for larger disturbance in feed (-10% -+10%) **Figure 6-10** shows the plot of loss by keeping three measurements constant and varying the feed flow rate. It is clear from the figure that the sets with rank1, rank2, rank3 and rank5 show nearly same loss (%) with varying feed. However, the set which was ranked 4th using local method gives worst loss. Also the temperature set which was ranked 1st gives minimum loss with respect to other measurement sets only for increase in feed flow rate. However with decreasing feed flow rate, the set of measurements (rank2) gives the minimum loss with respect to other sets of measurements.

The figure below shows the loss plot with varying feed for null space method. The null space method gave zero loss (both average and worst-case loss) using exact local method whereas on the non-linear model the loss is very high. It can be seen in the figure that the loss is approximately zero for very small decrease in feed flow rate however with increasing disturbance, the loss increases very sharply. The reason for poor performance in case of higher variation in feed flow rate is the non-linearity in the model. The measurement combinations from null space method is recommended to be used for very small disturbance in feed flow rate.

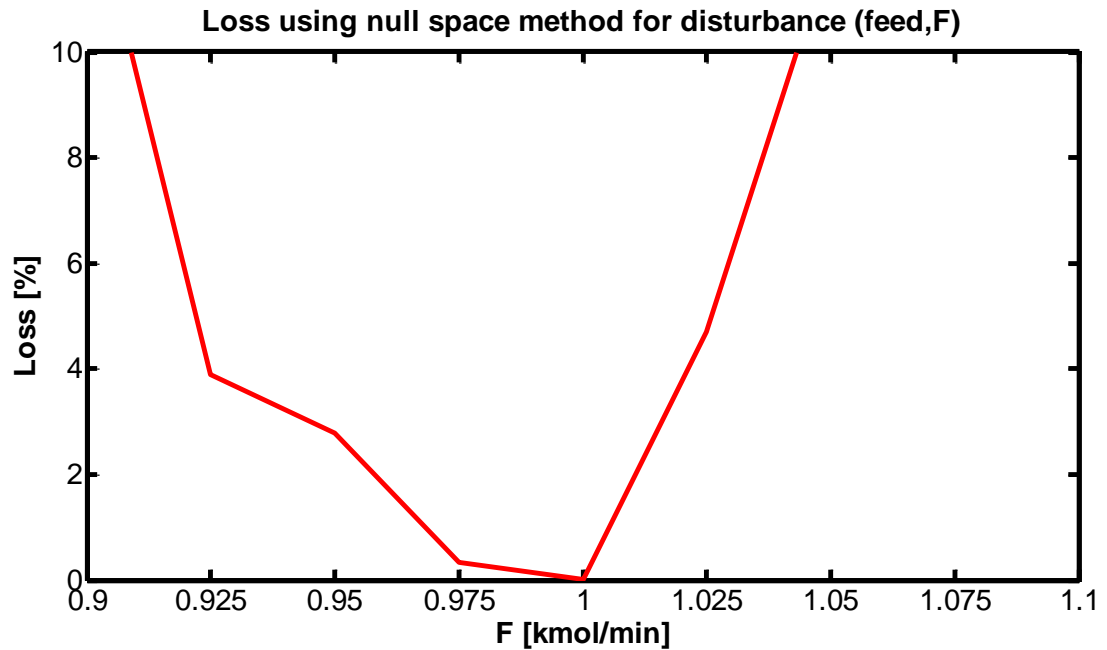


Figure 6-11 : The loss obtained from the non-linear model due to disturbance in feed for self-optimizing control by null space method

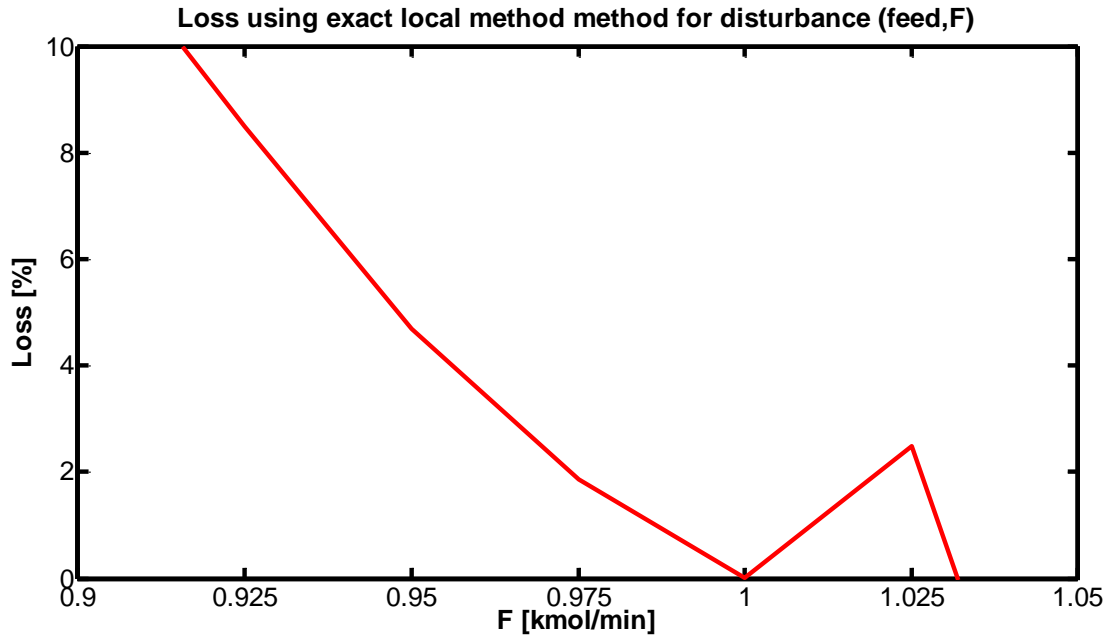


Figure 6-12 : The loss obtained from the non-linear model due to disturbance in feed for self-optimizing control by exact local method for all combination of measurements

The loss by keeping the measurement combinations obtained from exact local method also shows very poor performance for larger variation in feed. The exact local method is found to work well only in case of very small loss. The non-linearity in the model poorly affects the performance of self-optimizing control by keeping the measurement combinations obtained using exact local method.

6.8 Results from dynamic simulation

The physical locations of all set of temperatures given by **Eq. (6.12)** and **Eq.(6.13)** were nearly same and also the temperatures in each set are located in the same sections of the column. T_8 , T_9 , T_{10} and T_{11} are located in the first section of the column (the part of the prefractionator above feed stage) and is also close to liquid split ratio R_p . Similarly, T_{38} and T_{39} are located in the fourth section of the column (in the main column) and is also close to reflux, L . Likewise, T_{58} , T_{59} , T_{60} and T_{63} are located at the end of fifth section of

the column and is close to side stream, S . While T_{38} is the most preferred measurement and is present in almost all best sets of temperature. The minimum singular value method and the bi-directional branch and bound method by no means can make the selections based on the structural/section constraint. Neither do they give the measurements based on the controllability or stability analysis. However, in this case study it was found that all best sets of candidate controlled variables calculated by both methods gave the temperatures in each section and also close to remaining unconstrained degrees of freedom. This implies that these temperatures could be used to pair with unconstrained degrees of freedom both for self-optimizing control and stabilizing control. Since, there was not much variations in the values of loss by keeping these sets of measurement constant (except rank4 set containing T_{10} , T_{38} and T_{63}), all other sets of measurements could be used for economic self-optimizing control and stabilizing control. But for stabilizing control the RGA analysis was done at steady-state and the results of loss by the control configuration using one of these sets has been presented below

Pairing of controlled variables and unconstrained degrees of freedom: The result from steady-state analysis of the relative gain array for the control configuration using T_{10} , T_{38} , T_{60} as controlled variables and liquid split ratio R_l , reflux L and side stream S is given in **Table 6-9**. The RGA element should be preferably close to unity and also the pairing should be avoided for negative RGA element. Based on these criteria for pairing based on RGA, it is very that R_l should be paired with T_{10} , L should be paired with T_{38}

and S should be paired with T_{60} . The other sets of temperatures can also be evaluated using steady-state RGA analysis for stabilizing control.

Table 6-9: The steady-state RGA for the selected controlled variables

	L	S	R_I
T_{10}	-0.00026	1.05E-05	1.000252
T_{38}	0.989655	0.010629	-0.00028
T_{60}	0.010608	0.98936	3.17E-05

The loss evaluation using dynamic model: The control configuration for the pairing as obtained from steady-state RGA analysis was implemented on the three-product divided wall column. The control configuration is shown in **Figure 6-13**. The evaluation of loss was done by keeping the three temperatures constant by using decentralized feedback control and giving 10% change in each disturbance at a time. The effects on cost have been calculated for both increase in disturbances and decrease in disturbances by 10%. **Table 6-10** and **Table 6-11** show the mole fractions of key components in all three products and loss associated with various disturbances in the column.

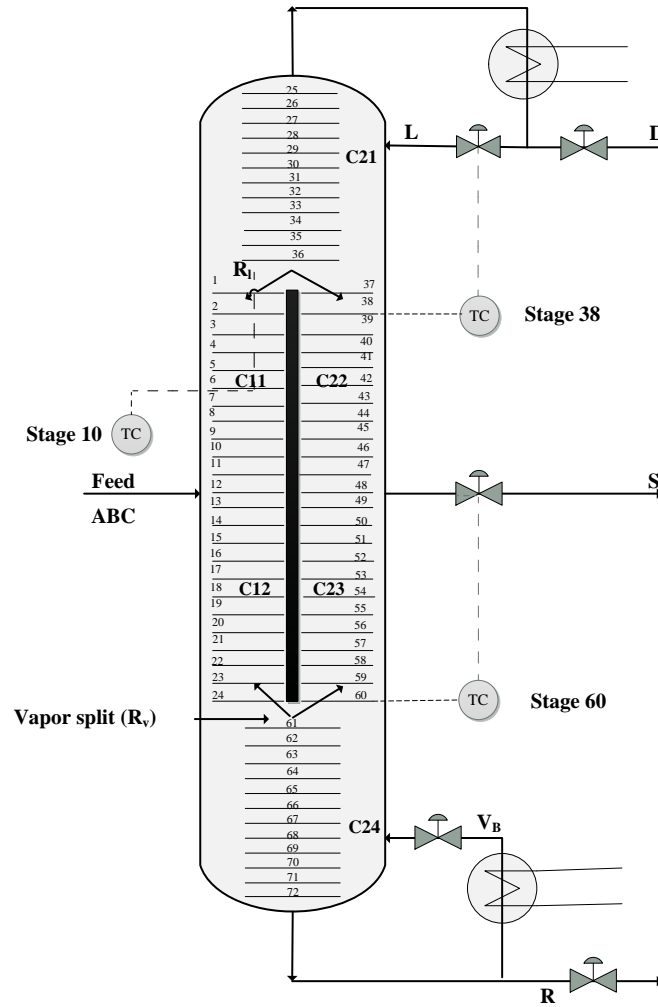


Figure 6-13: Self-optimizing control configuration (keeping three temperatures at their nominal setpoints using unconstrained degrees of freedom)

Table 6-10: The product purity compositions and percentage loss for +10% change in disturbances from nominal

	$x_{D,A}$	$x_{S,B}$	$x_{R,C}$	$J \times 10^{-3}$	$J_{opt,d} \times 10^{-3}$	Loss (%)
Nominal						
$F^* + 10\%$	0.996	0.9898	0.9972	6.3	6.100	3.278
$Rv^* + 10\%$	0.9962	0.9924	0.9981	4.418	4.300	2.730
$V^* + 10\%$	0.9977	0.9954	0.9988	2.723	2.600	4.718
$z_A^* + 10\%$	0.9956	0.9928	0.9987	4.402	4.087	7.710
$z_B^* + 10\%$	0.9967	0.9921	0.9986	4.442	4.350	2.104

Table 6-11: The product purity compositions and percentage loss for -10% change in disturbances from nominal

	$x_{D,A}$	$x_{S,B}$	$x_{R,C}$	J $\times 10^{-3}$	$J_{opt,d}$ $\times 10^{-3}$	Loss (%)
Nominal						
$F^* - 10\%$	0.997	0.9955	0.9988	2.386	2.300	3.742
$Rv^* - 10\%$	0.9975	0.9934	0.9983	3.617	3.605	0.466
$V^* - 10\%$	0.9958	0.9890	0.9970	6.051	5.900	2.564
$z_A^* - 10\%$	0.9979	0.9938	0.9975	3.632	3.493	3.779
$z_B^* - 10\%$	0.9972	0.9950	0.9979	3.194	3.15	1.406

CHAPTER 7

Conclusion and Further Work

7.1 Conclusion

The economic plantwide control procedure was applied to the three-product divided wall column. With four possible active constraints on the compositions of three key components in product streams and energy, the column can be optimally operated in 15 possible modes.

The maximum minimum singular value rule, minimum loss method (Halvorsen, Skogestad and Morud, et al. 2003) and null space method (Alstad and Skogestad 2007) were used to find the controlled variables that would minimize the loss caused due to deviation from optimal operation in self-optimizing control. Branch and bound method (Cao and Kariwala 2008) and bi-directional branch and bound methods (Kariwala, Cao and Janardhanan 2008) were also used to obtain best sets of candidate controlled variables using the above methods. It was found that, bi-directional branch and bound method using average loss criterion gave better sets of candidate controlled variables with less loss than that obtained from branch and bound method using maximum minimum singular rule. It was also found that the average loss calculated by using bi-directional branch and bound algorithm was slightly higher than the average loss calculated by using minimum loss method.

The steady-state loss by keeping all combinations of measurements (all 72 temperatures) at constant setpoints was less than that for three measurements (temperatures).

The results from non-linear steady-state model and dynamic model approved the selection of controlled variables done by steady-state exact local method for three measurements. However the results for all combinations of measurements were extremely poor for larger value of disturbances. Furthermore, the proposed control structure for one case seems to be good for self-optimizing control.

7.2 Further Work

In this work, selection of controlled variables was based on using maximum minimum singular value rule, minimum loss method (Halvorsen, Skogestad and Morud, et al. 2003) and null space method (Alstad and Skogestad 2007). These methods do not handle structural constraints therefore a mixed integer quadratic programming (MIQP) (Yelchuru 2012) method can be used to select optimal measurement subsets from each section. The model can be improved by working on its non-linearity as the loss evaluations from non-linear model for all combinations of measurements seemed not so good. For given sets of three measurements the loss evaluations using non-linear model should be done for the variation in remaining four disturbances (V_{\max} , R_1 , z_A and z_B) as this would give more informations which can be used in the better selection of controlled variables for self-optimizing control.

Also, the reported work can be implemented on the divided wall column in the experimental/industrial scale to check the validity of proposed work.

The present reported work was only for decentralized control structures. A comparison with multivariable controller could give very interesting result and insight in the proposed study.

In the proposed work mainly the steady state simulation was done to obtain the optimal controlled variable in self-optimizing control. It could be very interesting to extend the present work that result in economic optimal controlled variable based on rigorous dynamics simulations.

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APPENDIX A

Matlab Codes

Matlab Codes (Steady-state Simulation)

```
% Ambari Khanam
% contact at ambari.shams@hotmail.com

% Vmin digram (to create Vmin diagram Halvorsen's (Halvorsen 2001) codes were
used)

function [Vs,Ds,Rs,Keys,theta,VM,h]=UWmulti(theta,alfa,zf,qf,F,inkey,plotflag)
alfa = [4 2 1];
Zf = [0.333 0.333 0.333];
qF=1;
F=1;
function [Vs,Ds,Rs,Keys,theta,VM,h]=UWmulti([],alfa,zf,qf,F,[],1)

hold on

alfa = [4 2 1];
Zf = [0.53 0.13 0.333];
qF=1;
F=1;
function [Vs,Ds,Rs,Keys,theta,VM,h]=UWmulti([],alfa,zf,qf,F,[],1)

%initial steady state simulation (script name init_runner.m)

%initial steady state simulation
%% Three Product Petlyuk Column
%Constant Relative Volatility
% Initializes the model and runs
```

```

% The outputs are compositions (A, B and C) of (D, S, R, D1 and B1)
% Plot profiles give the composition profiles at steady-state
% Plot temperature profile gives temperature profile at steady-state.
% Petlyuk_NLmodel.m , compute_liquid.m, holdup_change.m, reboiler.m, gensec.m,
tank.m, and accum.m , indmat_Yes_S1 files should be in the same folder
%%
clear all; close all; clc;
global coldata dyndata hydraulic termodata UU alfa tend NI i
%% COLUMN DATA %%

% Number of stages in 6 sections of Petlyuk
coldata.Nt = [12 12 12 12 12 12];
% Initial holdup stages
coldata.M0 = [1 1 1 1 1 1 1 1 1 1 1];
% Boiling points of ethanol, propanol and n-butanol
coldata.Tboil = [78.37 97 117.4];
termodata.P = 1.0;
hydraulic.k1 = 1/0.063;
%% THERMODYNAMIC DATA %% (Realtive volatilities alfa)
alfa=[4.215374389 2.102194688 1] %ethanol propanol butanol

%% load nominal x u
load Nominal_final.mat % The nominal value obtained from optimization for ...
% minimizing the sum of impurities in the product streams (D, S and R)
UU=[]; %
i=0;% to initiate Petlyuk_openloop make change in CS by i+1
indmat_Yes_S1
% Make the nominal values of x, u and Temp global
dyndata.x_nom = x_nom;
dyndata.u_nom=u_nom;
dyndata.temp_nom=temp_nom;
%% Run this file to get initial values with LV Configuartion, uncomment
% line number
NI=5; % Number of integerators
options = odeset('MaxStep',10);
%tend=20000;
% at steady state reduce the end time to 5000
tend = 5000;
[t,x]=ode15s(@Simulation_Petlyuk,[0 tend],[dyndata.x_nom;zeros(NI,1)],options);
%% xf states to plot profiles.
xf=x(end,1:225)';
u_nom=UU(end,2:12)';
Plot_Profiles
dxdt = norm(Petlyuk_NLmodel(0, xf, u_nom));
% Print the values of compositions in D (distillate), S (side stream), R (residue)...
% and D1 and R1, (top and bottom product from the prefractionator both end)

```

```

dis_composition          % saved as init_compSS.mat
%Temperature as measurement Y
[sys Temp]= Petlyuk_NLmodel(t,xf,u_nom);
Yss = Temp;              % Steady-state Temperature, saved as Yss.mat
%plot_temp_profile      % Temperature Profile in the column,
%use command window to make temp profile

%%% The script file for indexing

%
% Index matrices
%There are six sections in the DWC; The order of stage numbering section
% wise is started from C11,C12 (Prefrac), C21,C22,C23,C24 (Main column),
%Refer to figure in the Master thesis by Ambari Khanam (2013)
%No. of stages in each section=12 (coldata.Nt=[12 12 12 12 12 12])
%No. of states in each section is 2*coldata.Nt(section), each section
%contains 24 states (12 for comp A and 12 for comp B) and then comes the
%next section.
global coldata
%states numbering in the prefractionator
im_x1 = 1:2 * coldata.Nt(1);          % 24 (12 for A and 12 for B) states in C11
(prefractionator)
im_x2 = im_x1(end) + [1:2 * coldata.Nt(2)]; %25-48 states in C12 (Prefrac)
% States numbering in the main column
im_x21 = im_x2(end) + [1:2 * coldata.Nt(3)]; %49-24*3=72 states in C21 (Main
column)
im_x22 = im_x21(end) + [1:2 * coldata.Nt(4)]; %73-24*4=96 states in C22
im_x23 = im_x22(end) + [1:2 * coldata.Nt(5)]; %97-24*5=120 states in C23
im_x24 = im_x23(end) + [1:2 * coldata.Nt(6)]; %111-24*6=144 states in C24
% States, Reboiler, condenser and side stream
im_xr = im_x24(end) + [1:2];          %145 146, comp A and B of reboiler stage
im_xt = im_xr(end) + [1:2];          %147, 148, of condenser
im_xS1 = im_xt(end) + [1:2];         %149,150, of side stream

%Holdups in the prefractionator
im_m1 = im_xS1(end) + [1:coldata.Nt(1)]; %150-162, trays holdups C11
im_m2 = im_m1(end) + [1:coldata.Nt(2)]; %163-174, trays holdups C12

%Holdups in the main column
im_m21 = im_m2(end) + [1:coldata.Nt(3)]; %175-186, trays holdups C21
im_m22 = im_m21(end) + [1:coldata.Nt(4)]; %187-198, trays holdups C22
im_m23 = im_m22(end) + [1:coldata.Nt(5)]; %199-210, trays holdups C23
im_m24 = im_m23(end) + [1:coldata.Nt(6)]; %211-222, trays holdups C24
%Reboiler, tank and side stream holdups
im_mr = im_m24(end) + 1;             %223, Reboiler
im_mt = im_mr(end) + 1;              %224, Condenser tank

```

```

im_mS1 = im_mt(end) + 1;           %225, Side stream collector
%Reshape the matrix to get comp A and B on the same stage, further to use
%for temperature calculation
II1=reshape(im_x1,coldata.Nt(1),2);
II2=reshape(im_x2,coldata.Nt(2),2);
II3=reshape(im_x21,coldata.Nt(3),2);
II4=reshape(im_x22,coldata.Nt(4),2);
II5=reshape(im_x23,coldata.Nt(5),2);
II6=reshape(im_x24,coldata.Nt(6),2);

%%% The function file for the Petlyuk non-linear model is Petlyuk_NLmodel.m

%% main function
function [sys Temp] = Petlyuk_NLmodel(t,x,U)

global dyndata coldata

L = U(1); VB = U(2);
Rl=U(3);Rv=U(4);
S1=U(5);
F=U(6);
zF = U(7:8); qF = U(9);
D = U(10); B = U(11);

% x=(x(12:end));
Rv2=1; %No vapor side draw

% Index matrices
indmat_Yes_S1;

% Nominal Input Parameters
%L=dyndata.u_nom(1);           % Reflux rate
%VB=dyndata.u_nom(2);         % Boilup rate
%Rl=dyndata.u_nom(3);         % Liquid split fraction to feed tray side
%Rv=dyndata.u_nom(4);         % Vapour split fraction to feed tray side
%S=dyndata.u_nom(5);          % Sideproduct removal rate
%F=dyndata.u_nom(6);          % Feed flow rate
%zF=dyndata.u_nom(7:8);       % Feed composition for components 1:2
%qF=dyndata.u_nom(9);         % Feed liquid fraction

Tboil=coldata.Tboil;

```

```

xp1 = x(II1);
xp2 = x(II2);
xp3 = x(II3);
xp4 = x(II4);
xp5 = x(II5);
xp6 = x(II6);
xp1=[xp1 1-sum(xp1,2)];
xp2=[xp2 1-sum(xp2,2)];
xp3=[xp3 1-sum(xp3,2)];
xp4=[xp4 1-sum(xp4,2)];
xp5=[xp5 1-sum(xp5,2)];
xp6=[xp6 1-sum(xp6,2)];
xp=[xp1;xp2;xp3;xp4;xp5;xp6];
Temp=xp*Tboil';

```

% Compute liquid flows for each section downwards

```

L21 = compute_liquid(3,L,x(im_m21),dyndata.u_nom(1),dyndata.x_nom(im_m21));
L1 =
compute_liquid(1,L21(end)*(Rl),x(im_m1),dyndata.u_nom(1)*(dyndata.u_nom(3)),dynd
ata.x_nom(im_m1));
L22 = compute_liquid(4,L21(end)*(1-Rl),x(im_m22),dyndata.u_nom(1)*(1-
dyndata.u_nom(3)),dyndata.x_nom(im_m22));
L2 =
compute_liquid(2,L1(end)+F*qF,x(im_m2),dyndata.u_nom(1)*(dyndata.u_nom(3))+F*q
F,dyndata.x_nom(im_m2));
L23 = compute_liquid(5,L22(end)-S1,x(im_m23),dyndata.u_nom(1)*(1-
dyndata.u_nom(3))-(dyndata.u_nom(5)),dyndata.x_nom(im_m23));
L24 = compute_liquid(6,L23(end)+L2(end),x(im_m24),...
dyndata.u_nom(1)*(1-dyndata.u_nom(3))-
(dyndata.u_nom(5))+dyndata.u_nom(1)*(dyndata.u_nom(3))+F*qF,dyndata.x_nom(im_
m24));

```

% Compute vapour flows for each section

```

V24 = VB*ones(coldata.Nt(6),1);
V2 = V24(1)*(Rv)*ones(coldata.Nt(2),1);
V23 = V24(1)*(1-Rv)*ones(coldata.Nt(5),1);
V1 = (V2(1)+F*(1-qF))*ones(coldata.Nt(1),1);
V22 = V23(1)*Rv2*ones(coldata.Nt(4),1);
V21 = (V22(1)+V1(1))*ones(coldata.Nt(3),1);

```

% Change in holdup

```

dm21 = holdup_change(L21,V21,L,V22(1)+V1(1));
dm1 = holdup_change(L1,V1,L21(end)*(Rl),V2(1)+F*(1-qF));

```

```

dm22 = holdup_change(L22,V22,L21(end)*(1-R1),V23(1)*Rv2);
dm2 = holdup_change(L2,V2,L1(end)+F*qF,V24(1)*(Rv));
dm23 = holdup_change(L23,V23,L22(end)-S1,V24(1)*(1-Rv));
dm24 = holdup_change(L24,V24,L23(end)+L2(end),VB);

% Change in compositions and temperatures
% Find vapour compositions for first two stages in the section and liquid
% composition of last stage
yr = reboiler(t,[x(im_xr); x(im_mr)],[], VB,3);
y1 = gensec(t,[x(im_x1); x(im_m1)],[],3,L1,V1,coldata.Nt(1));
y2 = gensec(t,[x(im_x2); x(im_m2)],[],3,L2,V2,coldata.Nt(2));

y21 = gensec(t,[x(im_x21); x(im_m21)],[],3,L21,V21,coldata.Nt(3));
y22 = gensec(t,[x(im_x22); x(im_m22)],[],3,L22,V22,coldata.Nt(4));
y23 = gensec(t,[x(im_x23); x(im_m23)],[],3,L23,V23,coldata.Nt(5));
y24 = gensec(t,[x(im_x24); x(im_m24)],[],3,L24,V24,coldata.Nt(6));

%find the derivatives
[dxr,dmr] = reboiler(t,[x(im_xr);x(im_mr)], [L24(end); y24(5:6); VB; B],1);
[dxt,dmt] = tank(t,[x(im_xt); x(im_mt)], [L; D; V21(1); y21(1:2)],1);

[dx1] = gensec(t,[x(im_x1); x(im_m1)], [L21(end)*(R1); y21(5:6); V2(1) + (1 - qF) * F;
(F*(1-qF)*zF+V2(1)*y2(1:2))/V1(end)],1,L1,V1,coldata.Nt(1));
[dx2] = gensec(t,[x(im_x2); x(im_m2)], [L1(end) + qF * F; (L1(end) * y1(5:6) + zF *
F*qF)/L2(1);(Rv) * V24(1); y24(1:2)],1,L2,V2,coldata.Nt(2));

[dx21] = gensec(t,[x(im_x21); x(im_m21)], [L; y21(1:2); V22(1)+V1(1);
(V1(1)*y1(1:2)+V22(1)*y22(1:2))/V21(end)],1,L21,V21,coldata.Nt(3));
[dx22] = gensec(t,[x(im_x22); x(im_m22)], [L21(end)*(1-R1); y21(5:6);Rv2 * V23(1);
y23(1:2)],1,L22,V22,coldata.Nt(4));
[dx23] = gensec(t,[x(im_x23); x(im_m23)], [L22(end)-S1; x(im_xS1);(1-Rv) * V24(1);
y24(1:2)],1,L23,V23,coldata.Nt(5));
[dx24] = gensec(t,[x(im_x24); x(im_m24)], [L2(end)+L23(end); (L2(end) * y2(5:6) +
L23(end) * y23(5:6))/L24(1);VB; yr'],1,L24,V24,coldata.Nt(6));

[dxS1,dmS1] = accum(t,[x(im_xS1); x(im_mS1)], [L22(end); y22(5:6); L23(1) + S1],1);

dm= [dm1;dm2;dm21;dm22;dm23;dm24];
dx = [dx1; dx2;dx21;dx22;dx23;dx24];
%sys is a column matrix with all the derivatives of compositions and
%holdups

sys = [dx; dxr; dxt;dxS1;dm; dmr; dmt;dmS1];

```



```
return;
```

% Compute liquid flows for a section

```
function L = compute_liquid(secnr,L_in,x,LO,xO)
global coldata hydraulic
i=1:coldata.Nt(secnr);L(i) = LO + (x(i)-xO(i))*hydraulic.k1 ;
L=L';
```

% Compute vapour flows for a section using heat loss and vapour bypassing

```
function V = compute_vapour(secnr,V_in,x)

global coldata termodata

temp = x;

V_heatloss = termodata.U * pi * coldata.diameter * ...
    coldata.sech(secnr) * (temp - termodata.T0) ...
    ./ (coldata.Nt(secnr) * termodata.deltaH);

V = [
    zeros(coldata.Nt(secnr),1)
    V_in
    ];
for k = coldata.Nt(secnr):-1:1
    V(k,1) = (1 - termodata.alpha) * V(k + 1,1) + ...
        termodata.alpha * V(k + 2,1) + ...
        V_heatloss(k,1);
end

V = V(1:coldata.Nt(secnr));
```

% Reboiler model

```
function [sys,dm] = reboiler(t,x,u,flag)

holdup = x(3);
x = x(1:2);

if (flag == 1)
    L_in = u(1);
    x_in = u(2:3);
```

```

V_out = u(4);
B = u(5);

% Derivatives
dm = L_in - V_out - B;
y = termo(x',3);
dx = (L_in * (x_in - x) - V_out * (y' - x)) / holdup;
sys = dx;
elseif (flag == 3)
% Measurements
[y] = termo(x',3);
sys = y;
end

% Tank model

function [sys,dm] = tank(t,x,u,flag)

holdup = x(3);

L = u(1);
D = u(2);
V_in = u(3);
x_in = u(4:5);

if (flag == 1)
% Derivatives

dm = V_in - L - D;
dx = (V_in * (x_in - x(1:2)))/holdup;
sys = dx;
elseif (flag == 3)
% Measurements

sys = x;
end

%This model is for Steady-state Simulations

function xprime=Simulation_Petlyuk(t,X)
%This model is for simulations
%This is a dynamic model with PI controllers, It returns derivative
% using the basic non-linear model Petlyuk_dxdt and it can be used for both
%steady-state simulation as well as dynamic simulations

```

```

%At steady state au=0 (except for condensers and reboiler holdups as they
%don't have steady-state effect)
%using this model simulations have been done to obtain steady state-gain
%for input and disturbances (Gy, Gyd)
%using this model simulations have been done to obtain Juu
%using this model dynamic simulations have been done for sequential
%controller tuning one by one by keeping au=0 or 1
%How? Just call the above function with different script files
%1. for initial steady state simulation with LV configuration the
% script file is      : init_sim_Petlyuk.m
%2. to calculate Gy and Gyd : script gains_Petlyuk.m
%3. to calculate Juu      : script Juu_Petlyuk.m
%4. for dynamic simulation : script file dynamic_Petlyuk.m
global UU dyndata tend NI i coldata
indmat_Yes_S1
Tboil=coldata.Tboil;
%better approximation for step size with some algorithm write in further
%work or discussion
%Delta1 = 1e-6;      %uncomment and use this perturbation in L and S1 to obtain Juu,
%
%Delta2= 1e-5;      %uncomment and use this perturbation in RI to obtain Juu

    Xp1 = X(II1);
    Xp2 = X(II2);
    Xp3 = X(II3);
    Xp4 = X(II4);
    Xp5 = X(II5);
    Xp6 = X(II6);
    Xp1=[Xp1 1-sum(Xp1,2)]; % compositions A, B and C in section 1
    Xp2=[Xp2 1-sum(Xp2,2)]; % compositions A, B and C in section 2
    Xp3=[Xp3 1-sum(Xp3,2)]; % compositions A, B and C in section 3
    Xp4=[Xp4 1-sum(Xp4,2)]; % compositions A, B and C in section 4
    Xp5=[Xp5 1-sum(Xp5,2)]; % compositions A, B and C in section 5
    Xp6=[Xp6 1-sum(Xp6,2)]; % compositions A, B and C in section 6
    Xp=[Xp1;Xp2;Xp3;Xp4;Xp5;Xp6];% Compositions A, B and C in the column
starting
                                % from section 1 and ending at section6
    Temp=Xp*Tboil';           % Temperatures on all stages sections (1,2,3,4,5,6)

% D and B used to control hold ups in the condenser (X(im_mt)) and reboiler
% (X(im_mr))respectively

[D,e1] = Controller_PI(X(im_mt),dyndata.x_nom(im_mt),dyndata.u_nom(end-
1),X(im_mS1+1),-1,1001,0,2);
[B,e2] =

```

```
Controller_PI(X(im_mr),dyndata.x_nom(im_mr),dyndata.u_nom(end),X(im_mS1+2),-
1,1001,0,2);
```

```
au=0; %(au=0 means controller is open and no control)
```

```
% Gy can be calculated here by giving step change in inputs (L, S and Rl) here.
```

```
[L,e3] = Controller_PI(Temp(38),(dyndata.temp_nom(38)),...
dyndata.u_nom(1),X(im_mS1+3),0.48*au/2,40*2,0,4);
```

```
% step change in L by adding 1e-6
```

```
% [L,e3] = Controller_PI(log(X(im_xt(2))),log(dyndata.x_nom(im_xt(2))),...
% dyndata.u_nom(1)-Delta1,X(im_mS1+3),0.48*au/2,40*2,0,4);
```

```
[S1,e4] = Controller_PI(Temp(42),dyndata.temp_nom(42),...
dyndata.u_nom(5),X(im_mS1+4),88*au/8,40*8,0,4);
```

```
% step change in S1, i.e.dyndata.u_nom(5)+1e-6
```

```
% [S1,e4] = Controller_PI(log((X(im_xS1(2))),log((dyndata.x_nom(im_xS1(2))),...
% dyndata.u_nom(5)-Delta1,X(im_mS1+4),88*au/8,40*8,0,4);
```

```
[Rl,e5] = Controller_PI(log(1-sum(X(im_x1([1 1+coldata.Nt(1)]))),...
log(1-sum(dyndata.x_nom(im_x1([1 1+coldata.Nt(1)]))),...
dyndata.u_nom(3),X(im_mS1+5),-0.333*au,40,0,1);
```

```
% step change in Rl, i.e.dyndata.u_nom(3)+1e-3
```

```
% [Rl,e5] = Controller_PI(Temp(6),...
% dyndata.temp_nom(6),...
% dyndata.u_nom(3)+Delta2,X(im_mS1+5),-0.333*au,40,0,1);
```

```
VBB = dyndata.u_nom(2); % Boilup if fixed
```

```
RV = dyndata.u_nom(4); % RV is fixed
```

```
% loop to obtain the values of i/p and disturbances throughout simulation
```

```
% time
```

```
if(t>0.01 || rem(i,10)==0) || t==tend
```

```
% t
```

```
UU=[UU; t [L;VBB;Rl;RV;S1;dyndata.u_nom(6:9); D; B]'];
```

```
end
```

```
i=i+1;
```

```
% t
```

```
xprime=Petlyuk_NLmodel(t,X(1:end),[L;VBB;Rl;RV;S1;dyndata.u_nom(6:9); D; B ]);
```

```
xprime=[xprime;e1;e2;e3;e4;e5];
```

%PI controller with saturation

```
function [u,e] = Controller_PI(T,Ts,u0,y,Kc,taui,min,max)
```

```
%PI controller with saturation
```

```

e=-T+Ts; eint=y;
u = u0 + Kc*e + (Kc/taui)*eint;

if u<min
    u=min;
elseif u>max
    u=max;
end

```

Matlab Codes for Self-optimizing Control

```

% Main Optimization file (script file Optimizer_Petlyuk.m)

% Main Optimization file
clear all; close all; clc;
% This is a script file for optimization
% The related script files with this file are Objective.m, Petlyuk_nonlcon
% (inequality constraints),Petlyuk_NLmodel(non-linear model)
% Other script files, .....are based on this main optimization
% file
% Global datas used are stages in the column, initial holdups in reboiler
% and condensers, boiling points of comp A, B and C, relative volatilities,
% thermal data and they are stored in structures coldata, dyndata, and
% hydraulic and termodata
%Nominal_final.mat has nominal values of composition, inputs and
%temperature
% Also the nominal states and input values (Nominal_final.mat) are made global
% by using dyndata as they are used as reference point for steady state
% simulation and also as setpoints for dynamic simulations

global coldata dyndata hydraulic alfa

% COLUMN DATA %%
% Number of stages in each section (C11,C12,C21,C22,C23,C24)
coldata.Nt = [12 12 12 12 12 12];
% Initial holdup in reboiler and condenser
coldata.M0 = [1 1 1 1 1 1 1 1 1 1];
% Boiling points of ethanol, propanol and n-butanol
coldata.Tboil = [78.37 97 117.4];

```

```

%Hydraulics
hydraulic.k1 = 1/0.063;

%Relative volatilit of Ethanol, Propanol and n-Butanol with respect to the
%heaviest n-Butanol
alfa=[4.215374389 2.102194688 1];

% Initial values for optimization made global
%load opt_init.mat
load Nominal_final

dyndata.x_nom = x_nom;
dyndata.u_nom = u_nom;
%dyndata.temp_nom = temp_nom;
options = optimset('fmincon');
options = optimset(options,'TolFun',1e-10,'TolCon',1e-
13,'MaxFunEvals',50000,'Display','none',...
'Algorithm','active-set');%,'Diagnostic','off');%,'GradObj','on','Hessian','on');%,...

% All the equality and inequality linear constraints are given in the file
% specs
Specs

% Optimization command
[x_opt,fval,exitflag,output,lambda,Grad,Hessian] = fmincon(@(x)
Objective(x),[x_nom;u_nom],Ain,bin,Aeq,beq,[],[],@(x) Petlyuk_nonlcon(x),options);

x_nom=x_opt(1:225);u_nom=x_opt(226:end);

dxdt = norm(Petlyuk_NLmodel(0,x_nom, u_nom));

xf=x_nom;
% script file for plotting composition profiles at the end of each
% optimization
Plot_Profiles
% script file for plotting temperature at the end of each optimization
%plot_temp_profile
% print selected variables or outputs, temperature or composition
%fval
% get temperatures
%[sys Temp]=Petlyuk_NLmodel([],xf,u_nom);
%Temp = sys(end-71:end);
%Y0= Temp;

```

```
% print the composition at the end of each optimization
[x_nom(im_xt(1)),x_nom(im_xt(2)),1-x_nom(im_xt(1))-x_nom(im_xt(2));...
 x_nom(im_xS1(1)),x_nom(im_xS1(2)),1-x_nom(im_xS1(1))-x_nom(im_xS1(2));...
 x_nom(im_xr(1)),x_nom(im_xr(2)),1-x_nom(im_xr(1))-x_nom(im_xr(2));...
 x_nom(im_x1(1)),x_nom(im_x1(coldata.Nt(1)+1)),1-x_nom(im_x1(1))-
x_nom(im_x1(1+coldata.Nt(2)));...
 x_nom(im_x2(coldata.Nt(2))),x_nom(im_x2(2*coldata.Nt(2))),1-x_nom(im_x2...
 (coldata.Nt(2)))-x_nom(im_x2(2*coldata.Nt(2)))]
```

```
% The results from optimization are saved in Nominal_final.mat
```

```
petlyuk_cost
```

%%% Non-linear equality and inequality constraints

```
function [c ceq]=Petlyuk_nonlcon(x)
global dyndata coldata
load Nominal_final1.mat
dyndata.temp_nom = temp_nom;
%Non linear equality and inequality constraints for optimization
%indmat_Yes_S1
%load Hel_halfdegree
%load csel_halfdegree
%load Hel3
% load csel3
%load H1ns
%load Csns
% load Hel
% load csel
U=zeros(11,1);
U(1:11)=x(226:236);           %inputs
s=x(1:225);                   %states

[xprime Temp] = (Petlyuk_NLmodel([],s,U));
ceq=xprime;                   % when no SOC

% ceq for 1st best temperature set using maximum minimum singular value
%ceq=[ xprime;Temp(10)-dyndata.temp_nom(10);Temp(38)-
dyndata.temp_nom(38);Temp(60)-dyndata.temp_nom(60)];
% ceq for 2nd best temperature set using maximum minimum singular value
%ceq=[ xprime;Temp(9)-dyndata.temp_nom(9);Temp(38)-
dyndata.temp_nom(38);Temp(60)-dyndata.temp_nom(60)];
% ceq for 3rd best temperature set using maximum minimum singular value
%ceq=[ xprime;Temp(11)-dyndata.temp_nom(11);Temp(38)-
```

```

dyndata.temp_nom(38);Temp(60)-dyndata.temp_nom(60)];
%ceq for 4th best temperature set using maximum minimum singular value
%ceq=[ xprime;Temp(10)-dyndata.temp_nom(10);Temp(38)-
dyndata.temp_nom(38);Temp(63)-dyndata.temp_nom(63)];
%ceq for 5th best temperature set using maximum minimum singular value
%ceq=[ xprime;Temp(8)-dyndata.temp_nom(8);Temp(38)-
dyndata.temp_nom(38);Temp(60)-dyndata.temp_nom(60)];
%ceq for 6th best temperature set using maximum minimum singular value
%ceq=[ xprime;Temp(9)-dyndata.temp_nom(9);Temp(38)-
dyndata.temp_nom(38);Temp(63)-dyndata.temp_nom(63)];
%ceq for 7th best temperature set using maximum minimum singular value
%ceq=[ xprime;Temp(7)-dyndata.temp_nom(7);Temp(38)-
dyndata.temp_nom(38);Temp(60)-dyndata.temp_nom(60)];
%ceq for 8th best temperature set using maximum minimum singular value
%ceq=[ xprime;Temp(10)-dyndata.temp_nom(10);Temp(38)-
dyndata.temp_nom(38);Temp(59)-dyndata.temp_nom(59)];
% ceq for 20th best temperature set using maximum MSV
%ceq=[ xprime;Temp(11)-dyndata.temp_nom(11);Temp(38)-
dyndata.temp_nom(38);Temp(64)-dyndata.temp_nom(64)];
% based on branch and bound method by Cao, the 1st set of three best
% temperatures based on bidirectional algorithm.
%ceq=[ xprime;Temp(43)-dyndata.temp_nom(43);Temp(60)-
dyndata.temp_nom(60);Temp(64)-dyndata.temp_nom(64)];
%ceq=[xprime;(Hel3*[Temp(10,1);Temp(38,1);Temp(60,1)])-csel3];
% Null space method
%ceq=[xprime;(H1ns*Temp-Csns)];
%Exact local method
%ceq=[xprime;(Hel*Temp-csel)];
c = []; %non linear inequality constraints

%%% Linear equality and inequality constraints (Petlyuk_nonlcon.m)
Specs, linear equality and inequality constraints
global dyndata

indmat_Yes_S1

Nz = size([dyndata.u_nom;dyndata.x_nom]);% all decision variables including inputs U
and compositions and holdup on stages

%Feed rate, composition & quality

```



```

Nv=6;
Aeq=zeros(Nv,Nz);beq=zeros(Nv,1); %linearity constraints where Ns are product/feed
specifications

% These are the values of only As which contributes in specifications and
% thus=1 and not 0.

Aeq(1,im_mS1+6)=1;           %feed flow rate, F (im_mS1+6), 231
Aeq(2,im_mS1+7)=1;           %composition of A in the feed, zF, (im_mS1+7),232
Aeq(3,im_mS1+8)=1;           %composition of B in the feed, zF, im_mS1+8),233
Aeq(4,im_mS1+9)=1;           %feed liquid fraction qf, (im_mS1+9),234
Aeq(5,im_mS1+2)=1;           %Boilup, Vmax, (im_mS1+4), 227

%beq(1:4)=dyndata.u_nom([6:9]);
beq(1)= dyndata.u_nom(6);     %Feed flow rate value (dd1)
beq(2)=dyndata.u_nom(7);     %Feed composition zA
beq(3)=dyndata.u_nom(8);     %Feed composition zB
beq(4)=dyndata.u_nom(9);     % liquid feed
beq(5)=dyndata.u_nom(2);     %The value of boilup Vmax (fixed)(dd3)
Aeq(6,im_mS1+4)=1;           % RV
beq(6)=0.95*dyndata.u_nom(4); % The value of vapor split ratio which is fixed
(dd5)

% Aeq (7,im_x1(1))=1;         % A in D1 (Prefrac top)
% Aeq(7,im_x1(coldata.Nt(1)+1))=1; % B in D1 (Prefrac top)
% 1+im_x1(coldata.Nt(1)+1)=1;
% beq(7)=1-0.003;           % C in D1 is (1-sum(A,B)) (This means active constraint)
% Aeq(7,47)=1;
% beq(7)=0.0015;%

%%%%%%%%%%
Ain=-eye(Nz,Nz);bin=zeros(Nz,1);%Non-negativity of state, helps optimizer

% Objective Function (@objective(x)

indmat_Yes_S1
% the disturbances are dT= [F zF Vmax RV ]
%The inputs are uT= [RI L s]

J=x(235)*x(148)+x(230)*(1-x(150))+x(236)*x(146); % minimize the sum of impurities

% Note: The value after optimization is saved as Nominal_final.mat and is

```

used as optimal values for all evaluations

```

%% Calculate F matrix (script name "script_Fmatrix)

% COLUMN DATA %%
% Pass the options for optimization
% Number of stages in each section (C11,C12,C21,C22,C23,C24)
coldata.Nt = [12 12 12 12 12 12];
% Initial holdup in reboiler and condenser
coldata.M0 = [1 1 1 1 1 1 1 1 1 1 1];
% Boiling points of ethanol, propanol and n-butanol
coldata.Tboil = [78.37 97 117.4];
% Hydraulics
hydraulic.k1 = 1/0.063;
% Relative volatility of Ethanol, Propanol and n-Butanol with respect to the
% heaviest component n-Butanol
alfa=[4.215374389 2.102194688 1];

% Optimization
% Re-optimize for disturbances (F, zA, zB, V, and RV)
% Load output temperature at the nominal values Y0
load Y0
% All linear equality and inequality constraints given in specs, the
% Disturbances can be directly set in specs file
% Specs
% Initial values for optimization made global
load Nominal_final.mat
dyndata.x_nom = x_nom;
dyndata.u_nom = u_nom;
dyndata.temp_nom = temp_nom;
options = optimset('fmincon');

```

```

options = optimset(options,'TolFun',1e-8,'TolCon',1e-
8,'MaxFunEvals',500000,'Display','iter',...
'Algorithm','active-set');

%
Specs
%disturbance in feed flow rate dd1
dd1=1e-5 ;           % perturbation in feed flow rate
beq(1)=dyndata.u_nom(6)+dd1;

%Run the optimization with disturbance in feed flow rate dd1 while
%keeping other values same, run the loop to plot profile for disturbance in
%feed
[x_opt,fval,exitflag,output,lambda,Grad,Hessian] = fmincon(@(x)
Objective(x),[dyndata.x_nom;dyndata.u_nom],Ain,bin,Aeq,beq,[],[],@(x)
Petlyuk_nonlcon(x),options);
%x_nom=x_opt(1:im_mS1);u_nom=x_opt(im_mS1+1:end);
x_nom=x_opt(1:225);u_nom=x_opt(226:end);   %It is same as above

dxdt = norm(Petlyuk_NLmodel(0,x_nom, u_nom));
[~, Temp]=Petlyuk_NLmodel(0,x_nom,u_nom);
ydd1= [Temp];

%disturbance in compositions zF1

beq(1)=dyndata.u_nom(6);   %Nominal feed same as before F0=1
dd2 = 1e-5;
%dd2=dyndata.u_nom(7)*0.2;
beq(2)=dyndata.u_nom(7)+dd2;

%Run the optimization with the disturbance in feed compositions

```

```

[x_opt,fval,exitflag,output,lambda,Grad,Hessian] = fmincon(@(x)
Objective(x),[dyndata.x_nom;dyndata.u_nom],Ain,bin,Aeq,beq,[],[],@(x)
Petlyuk_nonlcon(x),options);

x_nom=x_opt(1:225);u_nom=x_opt(226:end);

dxdt = norm(Petlyuk_Nlmodel(0,x_nom, u_nom));
[~, Temp]=Petlyuk_NLmodel(0,x_nom,u_nom);
ydd2= [Temp];

%disturbance in compositions zF2, B in feed
dd3= 1e-5;
beq(2)=dyndata.u_nom(7); %Nominal composition A
%dd3=dyndata.u_nom(8)*0.2;
beq(3)=dyndata.u_nom(8)+dd3;

%Run the optimization with the disturbance in feed compositions
[x_opt,fval,exitflag,output,lambda,Grad,Hessian] = fmincon(@(x)
Objective(x),[dyndata.x_nom;dyndata.u_nom],Ain,bin,Aeq,beq,[],[],@(x)
Petlyuk_nonlcon(x),options);

x_nom=x_opt(1:225);u_nom=x_opt(226:end);

dxdt = norm(Petlyuk_NLmodel(0,x_nom, u_nom));
[~, Temp]=Petlyuk_NLmodel(0,x_nom,u_nom);
ydd3= [Temp];

%Give disturbance in the Vmax (boilup) and make the last disturbance
%to the nominal
dd4=1e-5;
beq(3)=dyndata.u_nom(8);
%dd4=dyndata.u_nom(2)*0.1;
beq(5)= dyndata.u_nom(2)+dd4;

```

```

%Run the optimization with disturbance in the boilup but keeping other
%disturbances to the nominal
[x_opt,fval,exitflag,output,lambda,Grad,Hessian] = fmincon(@(x)
Objective(x),[dyndata.x_nom;dyndata.u_nom],Ain,bin,Aeq,beq,[],[],@(x)
Petlyuk_nonlcon(x),options);

x_nom=x_opt(1:225);u_nom=x_opt(226:end);

dxdt = norm(Petlyuk_NLmodel(0,x_nom, u_nom));
[~, Temp]=Petlyuk_NLmodel(0,x_nom,u_nom);
ydd4= [Temp];

% Change in RV
dd5 = 1e-5;
beq(5)=dyndata.u_nom(2);
%dd5=dyndata.u_nom(4)*0.1; %magnitude of perturbation in Rv 10 times
beq(6)=dyndata.u_nom(4)+dd5;

%Run the optimization
[x_opt,fval,exitflag,output,lambda,Grad,Hessian] = fmincon(@(x)
Objective(x),[dyndata.x_nom;dyndata.u_nom],Ain,bin,Aeq,beq,[],[],@(x)
Petlyuk_nonlcon(x),options);

x_nom=x_opt(1:225);u_nom=x_opt(226:end);

dxdt = norm(Petlyuk_NLmodel(0,x_nom, u_nom));
[sys Temp]=Petlyuk_NLmodel(0,x_nom,u_nom);
ydd5= [Temp];

% Calculate the sensitivity matrix F and store the value,
F1=[(ydd1-Y0)/dd1 (ydd2-Y0)/dd2 (ydd3-Y0)/dd3 (ydd4-Y0)/dd4 (ydd5-Y0)/dd5];

```

% Script for calculating gain matrix GY (w.r.t. input)**Script name GYscript.m**

```

clear all; close all; clc;
global coldata dyndata hydraulic termodata UU alfa tend NI i
%% COLUMN DATA %%

% Number of stages in 6 sections of Petlyuk
coldata.Nt = [12 12 12 12 12 12];
% Initial holdup stages
coldata.M0 = [1 1 1 1 1 1 1 1 1 1];
% Boiling points of ethanol, propanol and n-butanol
coldata.Tboil = [78.37 97 117.4];
termodata.P = 1.0;
hydraulic.k1 = 1/0.063;
%% THERMODYNAMIC DATA %%
alfa=[4.215374389 2.102194688 1] %ethanol propanol butanol

%% load nominal x u
load Nominal_final.mat % The nominal value obtained from optimization for ...
                        %minimizing the sum of impurities in the product streams (D, S and R)
UU=[];
i=0; %to initiate Petlyuk_openloop make change in CS by i+1
indmat_Yes_S1
% Initial values made global
dyndata.x_nom = x_nom;
dyndata.u_nom=u_nom;%
dyndata.temp_nom=temp_nom;
%% Run this file to get initial values with LV Configuartion, uncomment
% line number

```

```

NI=5; % Number of integerators
options = odeset('MaxStep',10);
tend=20000;
[t,x]=ode15s(@Simulation_Petlyuk,[0 tend],[dyndata.x_nom;zeros(NI,1)],options);
%% xf states to plot profiles.
xf=x(end,1:225)';
u_nom=UU(end,2:12)';
dxdt = norm(Petlyuk_NLmodel(0, xf, u_nom));
% Print the values of compositions in D (distillate), S (side stream), R (residue)...
%and D1 and R1, (top and bottom product from the prefractionator both end)
dis_composition
[sys Temp] = Petlyuk_NLmodel(tend, xf,u_nom);

% Optimal temperatures (measurement)also saved as temp_nom in
% Nominal_final.mat
load Y0.mat

%% Calculate steady state gain matrix for three remaining D.O.F. (L,S,RI) GY
%load Y0.mat
% Go to Petlyuk_openloop and give the step change in input L,uncomment line
% 53, 54
% and comment line 57, 58 dyndata.u_nom(1)+1e-5
%Run the simulation and store the value of Temp as YL
% YL= Temp;
%delL= 1e-5;
%dYdL = (YL-Y0)/delL;
load YL.mat
load dYdL.mat

%Give step change in S1, dyndata.u_nom(5)+1e-5
%Run the simulation and store the value of Temp as YS

```

```

%YS=Temp;
%delS= 1e-5;
%dYdS = (YS-Y0)/delS;
load YS.mat
load dYdS.mat

%Go to file Petlyuk_openloop and comment line number and uncomment line
%Give step change in RI, dyndata.u_nom(3)+1e-5
%Run the simulation and store the value of Temp as YRI
%YRI=Temp;
%delRI=1e-5;
%dYdRI = (YRI-Y0)/delRI;
load YRI.mat
load dYdRI.mat

%Steady state gain matrix GY (with respect to input)
GY = [dYdL dYdS dYdRI];

% Script for calculating gain matrix Gyd (w.r.t. disturbances)
Script file GYdscrip.m

clear all; close all; clc;
global coldata dyndata hydraulic termodata UU alfa tend NI i
%% COLUMN DATA %%

% Number of stages in 6 sections of Petlyuk
coldata.Nt = [12 12 12 12 12 12];
% Initial holdup stages
coldata.M0 = [1 1 1 1 1 1 1 1 1 1 1];
%Boiling points of ethanol, propanol and n-butanol
coldata.Tboil = [78.37 97 117.4];

```



```

termodata.P = 1.0;
hydraulic.k1 = 1/0.063;
%% THERMODYNAMIC DATA %%
alfa = [4.215374389 2.102194688 1]; %ethanol propanol butanol

%% load nominal x u
load Nominal_final.mat % The nominal value obtained from optimization for ...
%minimizing the sum of impurities in the product streams (D, S and R)
UU=[];
i=0; %to initiate Petlyuk_openloop make change in CS by i+1
indmat_Yes_S1
%Change in disturbances can be mase here to obtain Gyd
dyndata.x_nom = x_nom; %initial composition and holdup states
% disturbance in feed F, h=1e-5
h = 1e-5;
%dd1= h;
%u_nom(6)= u_nom(6)+dd1;
%disturbance in composition A in feed
%dd2=h;
%u_nom(7)=u_nom(7)+dd2;
%disturbance in composition B in feed
%dd3=h;
%u_nom(8)=u_nom(8)+dd3;

%disturbance in boilup
%dd4=h;
%u_nom(2)=u_nom(2)+dd4;

%disturbance in vapor split RV
%dd5=h;
%u_nom(4)=u_nom(4)+dd5;

```

```

dyndata.u_nom=u_nom;           %we have made initial input global
dyndata.temp_nom=temp_nom;
%% Run this file to get initial values with LV Configuartion, uncomment
% line number
NI=5; % Number of integerators
options = odeset('MaxStep',10);
tend=20000;
[t,x]=ode15s(@Simulation_Petlyuk,[0 tend],[dyndata.x_nom;zeros(NI,1)],options);
%% xf states to plot profiles.
xf=x(end,1:225)';
u_nom=UU(end,2:12)';
Plot_Profiles
dxdt = norm(Petlyuk_NLmodel(0, xf, u_nom));
% Print the values of compositions in D (distillate), S (side stream), R (residue)...
%and D1 and R1, (top and bottom product from the prefractionator both end)
%dis_composition
%Temperature as measurement Y
[sys Temp]= Petlyuk_Nlmodel(t,xf,u_nom);
% Yss = Temp;           % Measurements, Temperatures on all
%stages at steady state
%plot_temp_profile     % Temperature Profile in the column

%% Calculate steady state gain matrix for three remaining D.O.F. (L,S,R1) GY
load Y0.mat           % same as nominal temperature
% For the disturbance in feed flow rate F
%Run the simulation and store the value of Temp as YF
% YF= Temp;
%dYdF = (YF-Y0)/dd1;
load YF.mat

```

```
load dYdF.mat

%For disturbance in composition of A in feed, zA
%Run the simulation and store the value of Temp as YzA
% YzA = Temp;
% dYdzA = (YzA-Y0)/dd2;
load YzA.mat
load dYdzA.mat

%For disturbance in composition of B in feed, zB
%Run the simulation and store the value of Temp as YzB
% YzB = Temp;
% dYdzB = (YzB-Y0)/dd3;
load YzB.mat
load dYdzB.mat

%For disturbance in the boilup V
%Run the simulation and store the value of Temp as YV
% YV = Temp;
% dYdV = (YV-Y0)/dd4;
load YV.mat
load dYdV.mat

%For disturbance in the vapor split ratio RV
%Run the simulation and store the value of Temp as YV
% YRV = Temp;
% dYdRV = (YRV-Y0)/dd5;
load YRV.mat
load dYdRV.mat

% Calculate the steady state gain model for diturbances
```

```
GYd = [dYdF dYdzA dYdzB dYdV dYdRV];
```

```
% Load steady-state disturbance gain
```

```
%load GYd
```

%Script for calculating cost after simulation

Petlyuk_cost.m

```
% It has been used to calculate Juu and Jud
```

```
indmat_Yes_S1
```

```
% J is the objective function "sum of impurities in products"
```

```
J = u_nom(10)* xf(im_xt(2))+ u_nom(5)*(1-xf(im_xS1(2)))+u_nom(11)*xf(im_xr(2))
```

%Script for calculating Jud

Jud_Petlyuk.m

```
% Script for calculating Jud
```

```
clear all; close all; clc;
```

```
global coldata dyndata hydraulic termodata UU alfa tend NI i
```

```
%% COLUMN DATA %%
```

```
% Number of stages in 6 sections of Petlyuk
```

```
coldata.Nt = [12 12 12 12 12 12];
```

```
% Initial holdup stages
```

```
coldata.M0 = [1 1 1 1 1 1 1 1 1 1 1];
```

```
%Boiling points of ethanol, propanol and n-butanol
```

```
coldata.Tboil = [78.37 97 117.4];
```

```
termodata.P = 1.0;
```

```
hydraulic.k1 = 1/0.063;
```

```
%% THERMODYNAMIC DATA %%
```

```
alfa = [4.215374389 2.102194688 1]; %ethanol propanol butanol
```

```

%% load nominal x u
load Nominal_final.mat % The nominal value obtained from optimization for ...
% minimizing the sum of impurities in the product streams (D, S and R)
UU=[];
i=0; %to initiate Petlyuk_openloop make change in CS by i+1
indmat_Yes_S1
%Change in disturbances can be mase here to obtain Jud and also the input
%change has to be done in Simulation_Petlyuk.m
dyndata.x_nom = x_nom; %initial composition and holdup states
% disturbance in feed F, h=1e-5
h = 1e-5;
%dd1= h;
%u_nom(6)= u_nom(6)+dd1;
%disturbance in composition A in feed
%dd2=h;
%u_nom(7)=u_nom(7)+dd2;
%disturbance in composition B in feed
%dd3=h;
%u_nom(8)=u_nom(8)+dd3;

%disturbance in boilup
%dd4=h;
%u_nom(2)=u_nom(2)+dd4;

%disturbance in vapor split RV
%dd5=h;
%u_nom(4)=u_nom(4)+dd5;

dyndata.u_nom=u_nom; %we have made initial input global
dyndata.temp_nom=temp_nom;

```

```

%% Run this file to get initial values with LV Configuartion, uncomment
% line number
NI=5; % Number of integerators
options = odeset('MaxStep',10);
tend=20000;
[t,x]=ode15s(@Simulation_Petlyuk,[0 tend],[dyndata.x_nom;zeros(NI,1)],options);
%% xf states to plot profiles.
xf=x(end,1:225)';
u_nom=UU(end,2:12)';

%Script file to calculate cost after simulation
petlyuk_cost

%The matrix Jud is also saved in the matlab SS code
%load Jud

% Check Juu is positive definite or not
The script file is Juu_positivedefinite.m

Juu = [1709 -993.3114 -17.96;-993.3 114 1012.6 12.583;...
-17.96 12.583 1.8781];

%Script for checking positive definite of a matrix
[m,n]=size(Juu);
if m~=n,
    error('Juu is not Symmetric');
end

%Test for positive definiteness
x=1; %Flag to check for positiveness
for i=1:m
    subJuu=Juu(1:i,1:i); %Extract the upper left kxk submatrix

```

```

    if(det(subJuu)<=0); %Check wheather the determinent of the kxk submatrix is +ve
        x=0;
        break;
    end
end

% Exact Local Method applied to three-product DWC
clear all; close all; clc;

global coldata dyndata hydraulic termodata UU alfa
% COLUMN DATA %%

% The script for calculating F matrix
%Script_Fmatrix
load F1

% Write specs after script_Fmatrix otherwise result might change
%Specs
load Nominal_final.mat
dyndata.u_nom = u_nom;

%Run the optimization

%[x_opt,fval,exitflag,output,lambda,Grad,Hessian] = fmincon(@(x)
Objective(x),[dyndata.x_nom;dyndata.u_nom],Ain,bin,Aeq,beq,[],[],@(x)
Petlyuk_nonlcon(x),options);

%x_nom=x_opt(1:225);u_nom=x_opt(226:end);

% dxdt = norm(Petlyuk_NLmodel(0,x_nom, u_nom));
%[sys Temp]=Petlyuk_NLmodel(0,x_nom,u_nom);
% Yo= Temp;
load Y0 %Nominal Temperature
% Scaling of disturbances
% 10% devaiations in F, zA, zB, 20% in Vmax and 10% in RV
dd=[0.01*dyndata.u_nom(6);0.01*dyndata.u_nom(7);0.01*dyndata.u_nom(8);...
0.01*dyndata.u_nom(2);0.01*dyndata.u_nom(4)];
%scaled with respect to Vmax
Wnd= diag(dd);
%Measurement error
%del=0.1; %0.5 degree C
% Wn= 0.5*diag(ones(72,1));
Wn= 1*diag(zeros(72,1)); % without noise

```

```

%Finding steady state gain matrix for three inputs L, RI and S
%Run the file init_runner and obtain the value of GY as per instructions
load GY
% Y=[F1*Wnd Wn];
Y=[F1*Wnd Wn]; % without noise
Hel=(inv(Y*Y')*(GY))'; %3X72
csel=Hel*Y0;
% or the combination can be made with the selected measurement only
load Juu.mat;
%Juu =eye(3);
load Jud.mat;
load GYd.mat;
M = sqrtm(Juu)*inv(Hel*GY)*(Hel*Y)
% Average loss is calculate dusing frobenius norm
Lavg = 0.5* norm(M,'fro')^2
% 0.0548
% Worst case loss is calculated using induced 2 norm
Lwc = 0.5* norm(M,2)^2
% 0.

%Exact local method for the set of three temperatures obtained from branch
%and bound Cao & Kariwala 2008
% This method has been used here to prescreen the candidate controlled
% variables
% Exact Local Method applied to three-product DWC

clear all; close all; clc;

global coldata dyndata hydraulic termodata UU alfa
% COLUMN DATA %%k

% The script for calculating F matrix
%Script_Fmatrix % This gives an average loss 0.0455 and
load F1
%same as F1

load Nominal_final.mat
dyndata.u_nom = u_nom;

load Y0 %Nominal Temperature
% Scaling of disturbances
% 10% devaiitions in F, zA, zB, 10% in Vmax and 10% in RV
dd=[0.01*dyndata.u_nom(6);0.01*dyndata.u_nom(7);0.01*dyndata.u_nom(8);...
0.01*dyndata.u_nom(2);0.01*dyndata.u_nom(4)];
%scaled with respect to Vmax
Wnd= diag(dd);

```



```

%Measurement error
%0.5 degree C
Wn= 0.5*diag(ones(3,1));
% Wn= 1*diag(zeros(3,1));           % without noise

% sset = [10 38 60];           % 1st rank
% sset = [9 38 60];           % 2nd rank
% sset = [11 38 60];          % 3rd rank
% sset = [10 38 63];          % 4th rank
% sset = [8 38 60];           % 5th rank
% sset = [9 38 63];           % 6th rank
% sset = [7 38 60];           % 7th rank
% sset = [10 38 59];          % 8th rank
% sset = [13 38 62];          % 9th rank
% sset = [11 38 63];          % 10th rank

% The best ten sets of temperatures as obtained by average loss
% calculation by Cao and Kariwala
% sset = [9 38 59];           % 1st best
% sset = [9 38 58];           % 2nd best
% sset = [9 39 59];           % 3rd best
% sset = [39 57 63];          % 4th best
% sset = [9 39 58];           % 5th best
% sset = [8 38 59];           % 6th best
% sset = [8 38 58];           % 7th best
% sset = [8 39 59];           % 8th best
% sset = [10 39 59];          % 9th best
% sset = [10 38 58];          % 10th best

% Finding steady state gain matrix for three inputs L, RI and S
% Run the file init_runner and obtain the value of GY as per instructions
load GY
GY3 = GY(sset,:);
F3 = F1(sset,:);
Y3=[F3*Wnd Wn];               % without noise
Hel3=(inv(Y3*Y3')*(GY3))';    % 3X72
% csel3=Hel3*Y0(sset,:);
% or the combination can be made with the selected measurement only

% Evaluation of loss using exact local method
load Juu.mat;
%Juu =eye(3);
load Jud.mat;
%load GYd.mat;

```

```

M3 = sqrtm(Juu)*inv(Hel3*GY3)*(Hel3*Y3)

%M = sqrt([1861 0 0; 0 1160 0;0 0 1.84])*inv(Hel*GY)*Hel*Y
% Average loss is calculate dusing frobenius norm
Lavg = 0.5* norm(M3,'fro')^2
% 0.0548
% Worst case loss is calculated using induced 2 norm
Lwc = 0.5* norm(M3,2)^2
% 0.

%Minimum Singular Value Rule

%Scale the input using linear model such that each input has same effect on
%the cost J, get UscI,j= 1/(abs(Juu))^1/2, 3x1 matrix
%Load Juu.mat

clear all; close all; clc;

global coldata dyndata hydraulic termodata UU alfa

% The script for F matrix (optimal sensitivity)is script_Fmatrix

%script_Fmatrix

% instead of writing above script load F1 directly
load F1.mat
% The value of Juu as calculated using finite-diffrence approximation
% method

load Juu
u_sc = [1/sqrt(Juu(1,1)); 1/sqrt(Juu(2,2));1/sqrt(Juu(3,3))];

%optimal variation in candidate controlled variables w.r.t. disturbances
%load F1
dd1= 1e-5;dd2=1e-5;dd3=1e-5;dd4=1e-5;dd5=1e-5;
delYopt = F1*[dd1; dd2; dd3; dd4; dd5];

%for controlled variable which is temperature here , the implementaion
%error 0.5 degree C added, no control error because of PI controller
nm = 0.5*ones(72,1);
CscI = abs(delYopt)+nm;

%Scaling matrix for the controlled variables and inputs
Dc = diag(CscI);
Du = diag (u_sc);

```

```

% The scaled model
load GY
G = inv(Dc)*GY*Du;
%load G
%load Juu
%Jud=inf;
%Gd1=inf;
load Wn
load Wnd

% The branch and bound algorithm to calculate maximum of the minimum
% singular values to select the best combination of measurement which are
% three temperatures here.
%[B,sset,ops]=b3msv(Q,nc)
% G is scaled gain matrix (Ivar Halvorsen, Sigurd Skogestad, John Morud and
% V. Alstad Paper 2003,"optimal selection of controlled variables", INCER
% MSV saved as MSV and sset saved as sset, total 20 sets of measurements
[MSV,sset,ops]=b3msv(G,20);

% Calculate the loss using the value of B saved as MSV.mat(minimum singular
% values)

Loss_MSV = norm(Juu,2)*0.5*1/norm(G,2)^2
% The end of MSV

% RGA Calculation (pairing of T10, T38, T60 with L, S and RL)
load GY
Grga = [GY(10,:);GY(38,:);GY(60,:)];
R = inv(Grga') .* Grga ;
%Relative gain array is save as R, [-0.000336,1.88e-05,1.00031712216556;0.987
%,0.012,-0.000363;0.01268,0.9872,4.6528e-05];

%Null space method and slection of measurement sequential method
clear all; close all; clc;

global coldata dyndata hydraulic termodata UU alfa
% COLUMN DATA %%

% The script for calculating F matrix
%Script_Fmatrix
load F1
%load the nominal temperatures
load Y0
%u_sc = [1/sqrt(Juu(1,1)); 1/sqrt(Juu(2,2));1/sqrt(Juu(3,3))];

```

```

%GY0 = inv(Wn)*GY*u_sc;
%load GY0
% Find the maximum minimum singular value for all element of GY0
%GYsing = sort(abs(GY0));
% The best subset of measurement are ( T35, T34, T33) based on input only
% i.e. nu =3
% from best to worst
% The best subset of measurements are (T35, T34, T33, T36,T37,T10,T9, T38],
% nu+nd=ny i.e.3+5=8

H1 = null(F1');
H1=H1';
H1ns= H1(3,:);
Csns=H1ns*Y0;

```

Mtialab Codes for Dynamic Simulations

```

%% Three Product Petlyuk Column
%Constant Relative Volatility
% Initializes the model and runs
% The outputs are compositions (A, B and C) of (D, S, R, D1 and B1)
%%
clear all; close all; clc;
global coldata dyndata hydraulic termodata UU alfa tend NI i stages_Temperature
stages_Temperature_name Temp_nom
%% COLUMN DATA %%

% Number of stages in 6 sections of Petlyuk
coldata.Nt = [12 12 12 12 12 12];
% Initial holdup stages
coldata.M0 = [1 1 1 1 1 1 1 1 1 1 1];
%Boiling points of ethanol, propanol and n-butanol
coldata.Tboil = [78.37 97 117.4];
termodata.P = 1.0;
hydraulic.k1 = 1/0.063;
%% THERMODYNAMIC DATA %% (Realtive volatilities alfa)
alfa=[4.215374389 2.102194688 1] %ethanol propanol butanol

%% load nominal x u
load Nominal_final.mat % The nominal value obtained from optimization for ...

%minimizing the sum of impurities in the product streams (D, S and R)
UU=[]; %

```

```

i=0;%to initiate Petlyuk_openloop make change in CS by i+1
indmat_Yes_S1
% Make the nominal values of x, u and Temp global
dyndata.x_nom = x_nom;
%u_nom(6) =0.9*u_nom(6);
%u_nom(2) = 1.1*u_nom(2);
dyndata.u_nom=u_nom;
%dyndata.temp_nom=temp_nom;
%get stage indices for prefrac and main column
coldata.stages_pre=[im_x1(1:coldata.Nt(1)) im_x2(1:coldata.Nt(2))];
coldata.stages_main=[im_x21(1:coldata.Nt(3)) im_x22(1:coldata.Nt(4))
im_x23(1:coldata.Nt(5)) im_x24(1:coldata.Nt(6))];
%define position for temperature controller
stages_Temperature_name={'L','S1','RL'};
stages_Temperature=[im_x22(2) im_x23(12) im_x1(10)];
%calculate nominal temperature
Temp_nom=get_Temperature(stages_Temperature,1,dyndata.x_nom);
%% Run this file to get initial values with LV Configuration, uncomment
% line number
NI=5; % Number of integerators
options = odeset('MaxStep',10);
tend=5000;
[t,x]=ode15s(@Dynamic_Petlyuk,[0 tend],[dyndata.x_nom;zeros(NI,1)],options);
%% xf states to plot profiles.
xf=x(end,1:225)';
u_nom=UU(end,2:12)';

% Output at the end of simulation
Plot_Profiles
dxdt = norm(Petlyuk_NLmodel(0, xf, u_nom));
% Print the values of compositions in D (distillate), S (side stream), R (residue)...
%and D1 and R1, (top and bottom product from the prefractionator both end)
dis_composition % saved as init_compSS.mat
%Temperature as measurement Y
[sys Temp]= Petlyuk_NLmodel(t,xf,u_nom);
Yss = Temp; % Steady-state Temperature, saved as Yss.mat
%plot_temp_profile % Temperature Profile in the column,
%use command window to make temp profile
%Petlyuk_cost

function xprime=dynamic_Petlyuk(t,X)
% This model is for simulations
% This is a dynamic model with PI controllers, It returns derivative
% using the basic non-linear model Petlyuk_Nlmodel and it can be used for both

```

```

% steady-state simulation as well as dynamic simulations
% At steady state au=0 (except for condensers and reboiler holdups as they
% don't have steady-state effect)
% using this model simulations have been done to obtain steady state-gain
% for input and disturbances (Gy, Gyd)
% using this model simulations have been done to obtain Juu
% using this model dynamic simulations have been done for sequential
% controller tuning one by one by keeping au=0 or 1
% How? Just call the above function with different script files
% 1. for initial steady state simulation with LV configuration the
% script file is      : init_sim_Petlyuk.m
% 2. to calculate Gy and Gyd : script gains_Petlyuk.m
% 3. to calculate Juu      : script Juu_Petlyuk.m
% 4. for dynamic simulation : script file dynamic_Petlyuk.m
global UU dyndata tend NI i coldata au stages_Temperature Temp_nom
indmat_Yes_S1

% D and B used to control hold ups in the condenser (X(im_mt)) and reboiler
% (X(im_mr)) respectively

[D,e1] = Controller_PI(X(im_mt),dyndata.x_nom(im_mt),dyndata.u_nom(end-
1),X(226),-1,1001,0,2);
[B,e2] = Controller_PI(X(im_mr),dyndata.x_nom(im_mr),dyndata.u_nom(end),X(227),-
1,1001,0,2);

% get Temperatures for current timestep
Temp_current=get_Temperature(stages_Temperature,1,X);

% Controller
au=0;

[L,e3] = Controller_PI(Temp_current(1),Temp_nom(1),...
dyndata.u_nom(1),X(228),-0.15*1,16,0,4);

% [L,e3] = Controller_PI(Temp_current(1),Temp_nom(1),...
% dyndata.u_nom(1),X(228),-0.15,16,0,4);

[S1,e4] = Controller_PI(Temp_current(2),Temp_nom(2),...
dyndata.u_nom(5),X(229),0.27*1,11.2,0,4);

% [S1,e4] = Controller_PI(Temp_current(2),Temp_nom(2),...
% dyndata.u_nom(5),X(229),0.27,11.2,0,4);
[R1,e5] = Controller_PI(Temp_current(3),Temp_nom(3),...

```



```

%check if X is row vector, if yes: transform matrix and set time to "1"
if size(states,2)==1
    states=states';
    t=1;
end

%get number of section for each stage
for k=1:size(stage,2), %stage loop
    for i=1:6, %section loop
        if 2*sum(coldata.Nt(1:i))>=stage(k)
            section(k)=i;
            break
        end
    end
end
end

%calculate
for i=1:size(stage,2),%get single composition vector for stage i "t x [A B C]"
    composition=[states(t,stage(i)) states(t,stage(i)+coldata.Nt(section(i)))];
    composition=[composition 1-sum(composition,2)];
    %get single Temperature vector for stage i "t x Temp"
    Temp_stage = composition*[78.37 97 117.4]';
    %add Temp vector for stage i to previous stages
    Temp=[Temp Temp_stage];
end

% Temperature profile on stages in the prefractionator and the main column
%stage=1:48;
%stage1=stage(13:36);
%Temp_pre=Temp(1:24);
%plot(stage1,Temp_pre,'b')
%hold on
%Temp_main=Temp(25:72);
%plot(stage,Temp_main,'r')

%Plot Yopt (change in temp profile because of disturbances)
stage=1:48;
stage1=stage(13:36);
delYopt1 = z2(1:24);
plot(stage1,delYopt1,'b')
hold on
delYopt2=z2(25:72);

```



```
plot(stage,delYopt2,'r')
```